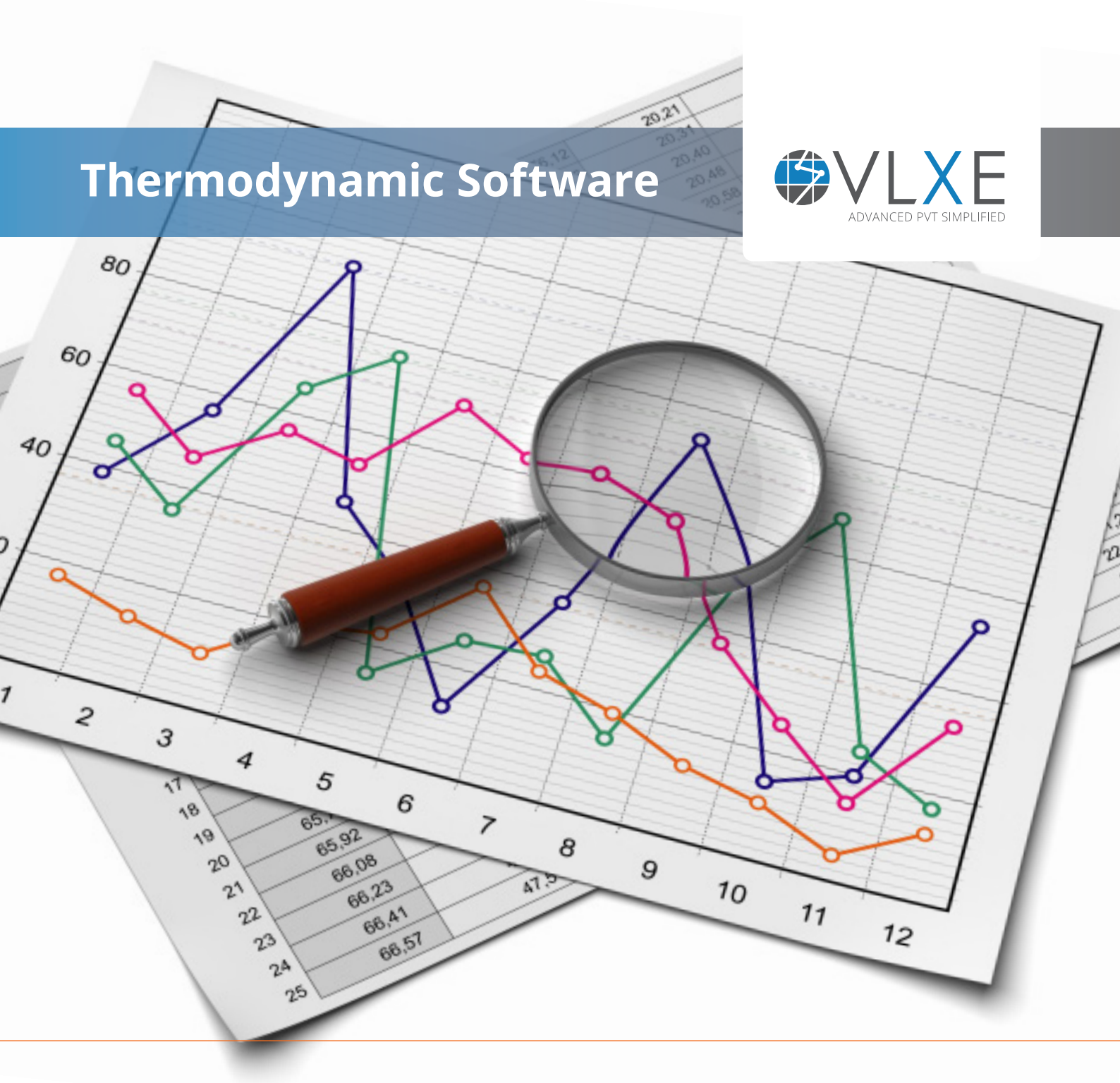
Thermodynamic Software

VLXE
ADVANCED PVT SIMPLIFIED



How to get started!

A complete guide to the VLXE Software

Version 2. August 2014

VLXE VLXE|BLEND®

www.vlxe.com

Thermodynamic Software

Table of Contents:

General information about the VLXE software

VLXE Software

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Written in Denmark, June 2014

1) Introduction

1.1 What can VLXE Blend Do?

VLXE Blend is a thermodynamic software package that is integrated into Excel. It provides a full range of PVT calculations inside Excel for a wide range of systems. The main focus is polymer and solvent systems, but it is also used for other systems with heavy components such as asphaltene systems. Customers looking to use PC-SAFT including associating and polar terms will similarly be fully covered by VLXE Blend. The VLXE API is not covered by this document.

1.2 How is this Documentation Organized?

A practical approach has been taken and two different set of sections are presented. First section (chapter 2) deals with the basic introduction to the software with simple examples. This includes calculation of cloud point and phase envelope both with binary components as well as more then two components. The chapters that follow each cover a feature of VLXE Blend.

1.3 Where to Start

If you are new user of VLXE Blend, you are advised to work through the entire second chapter. After that, pick and choose from the later chapters that are relevant for your needs.

1.4 Where to Find Additional Help

A help file is installed together with VLXE Blend. You can access it by selecting Support/Help under the VLXE Blend ribbon from inside Excel. The support webpage is also a great source of information:
http://www.vlxe.com/support

All VLXE customers are encouraged to contact VLXE for support. Your questions are always welcome!

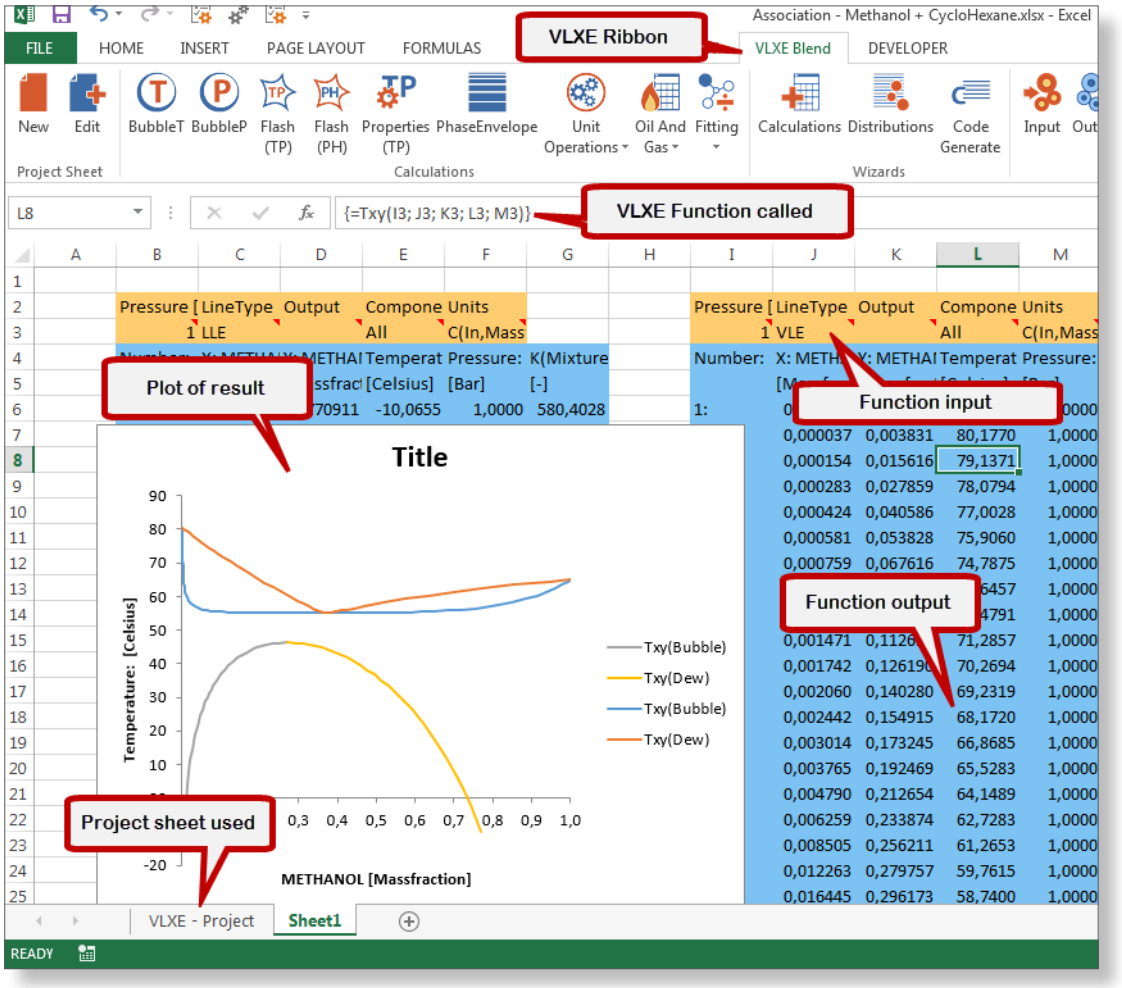
1.5 How to Proceed

Let's get started with the first section. Chapter 2 will show how to calculate cloud point and phase envelope for a simple mixture containing Methane and n-Hexane. Later examples are given with a mixture containing a few more components: methane, n-Hexane, n-octane and n-nonane. By working through this exercise, you will gain familiarity with the basic features of the package. Also you can get more practice by working on some advanced features of the software by following the examples given in the second section.

Some users may wish to jump right in and skip some (or all) of this tutorial. At any time whenever you are comfortable using the program, feel free to leave the tutorial and begin working on your own simulations.

2) Quick Overview

VLXE Blend integrates into Excel. The picture below highlights its 5 main features.



Ribbon:
Provides easy access to all features in VLXE Blend.

Function:
VLXE Blend performs all calculations using extra Excel functions.
They all work just like any other Excel function.

Function input:
Values given as input to the VLXE Blend Excel functions.

Function output:
Calculation results. They may be given in one or more cells.

Project sheet:
Is called before each calculation and holds all model and parameter information.

2.1 VLXE Blend in 10 seconds

- It integrates into Excel.
- It expands the standard functions found in Excel with the addition of thermodynamic functions.
- The VLXE Blend functions are like any other Excel function.
- All constant parameters used in a calculation are stored in the VLXE project sheet.
- Constants are taken from the VLXE Blend database and DIPPR database.
- Project sheets are created using a wizard.
- Calculations can be created by hand or using the wizard.
- All systems and calculations are handled the same way.
- Output is given either as a row or an area.
- The calculation engine can be used with in-house software using the API.

2.1.1 VLXE Blend basic rules

VLXE Blend covers a complete range of PVT calculations for a wide range of systems. But if you remember a few VLXE rules, you will find it very easy to use VLXE Blend, no matter how complex your system.

All calculations are used in the same way no-matter the type of system. Example: a flash calculation for an nhexane/Butane mixture is just as easy as for Ethylene/HDPE, even with 100 pseudo components.

The wizards included will make it easy to create a new calculation. However, since the VLXE Blend Excel functions work just like the built-in ones, you can also skip the wizards and create them yourself.

The VLXE database included can easily be edited using the tool provided. You can find it inside Excel, in the VLXE Ribbon under Support.

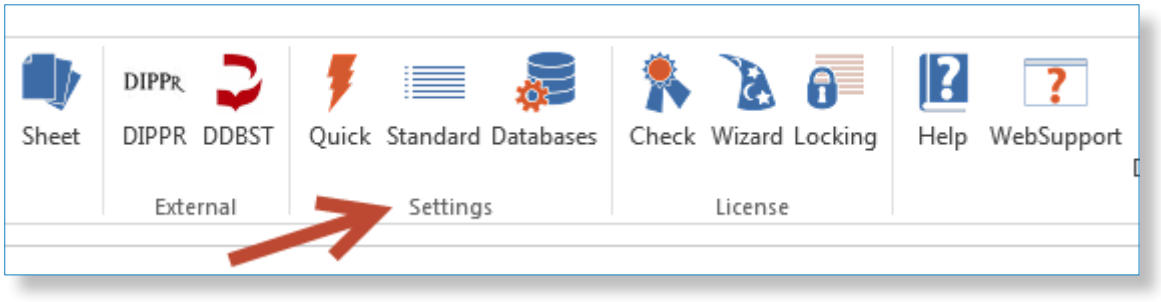
VLXE Blend supports the use of 2 databases. Personal and company wide. This allows a company to build an in-house parameter database that is available to all VLXE Blend users, while at the same time each user can have a private version.

2.1.2 Settings

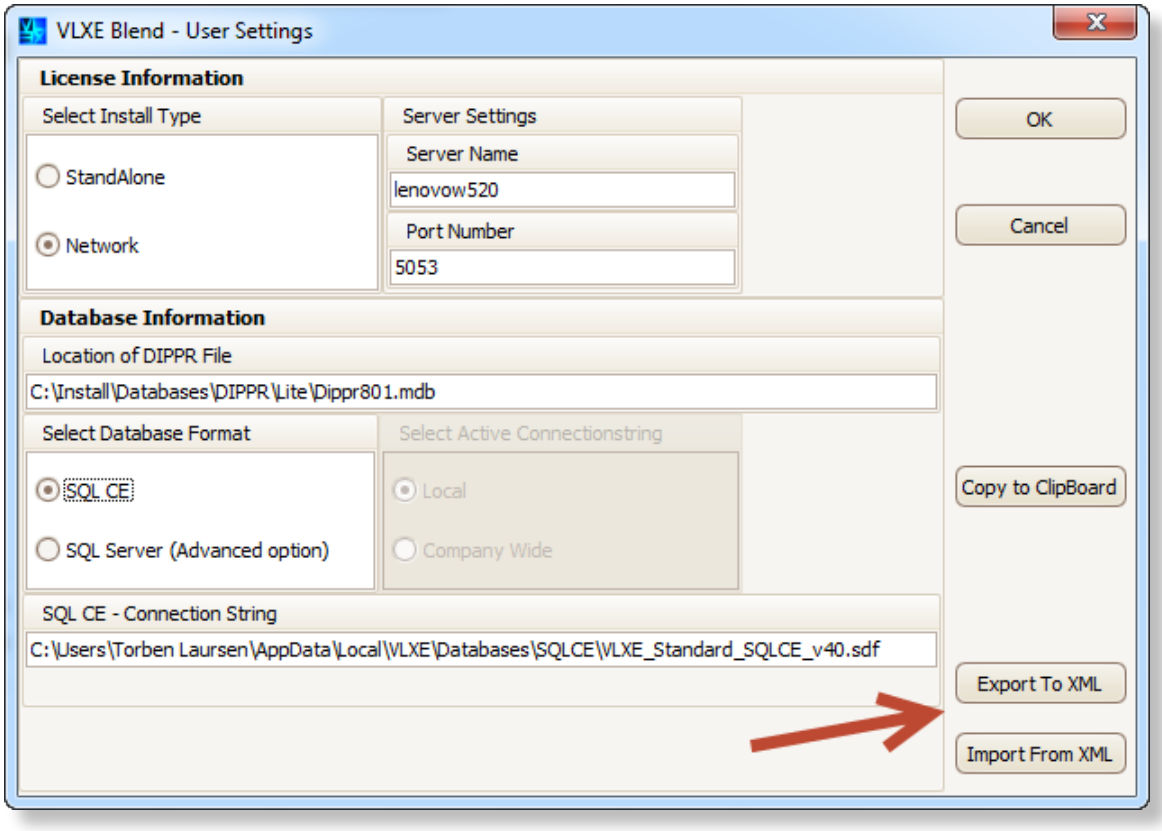
VLXE Blend requires you to set a few settings. They are set to default values when the software is installed. But can be changed at any time.

Three wizards are included to make it easy to work with the settings, these are:
- Quick.
- Standard
- Databases

You find shortcuts to all 3 on the VLXE Blend ribbon, under settings.



The “Quick” menu lets you quickly view and change the license and database settings. It also allows you to export and import settings, if needed.

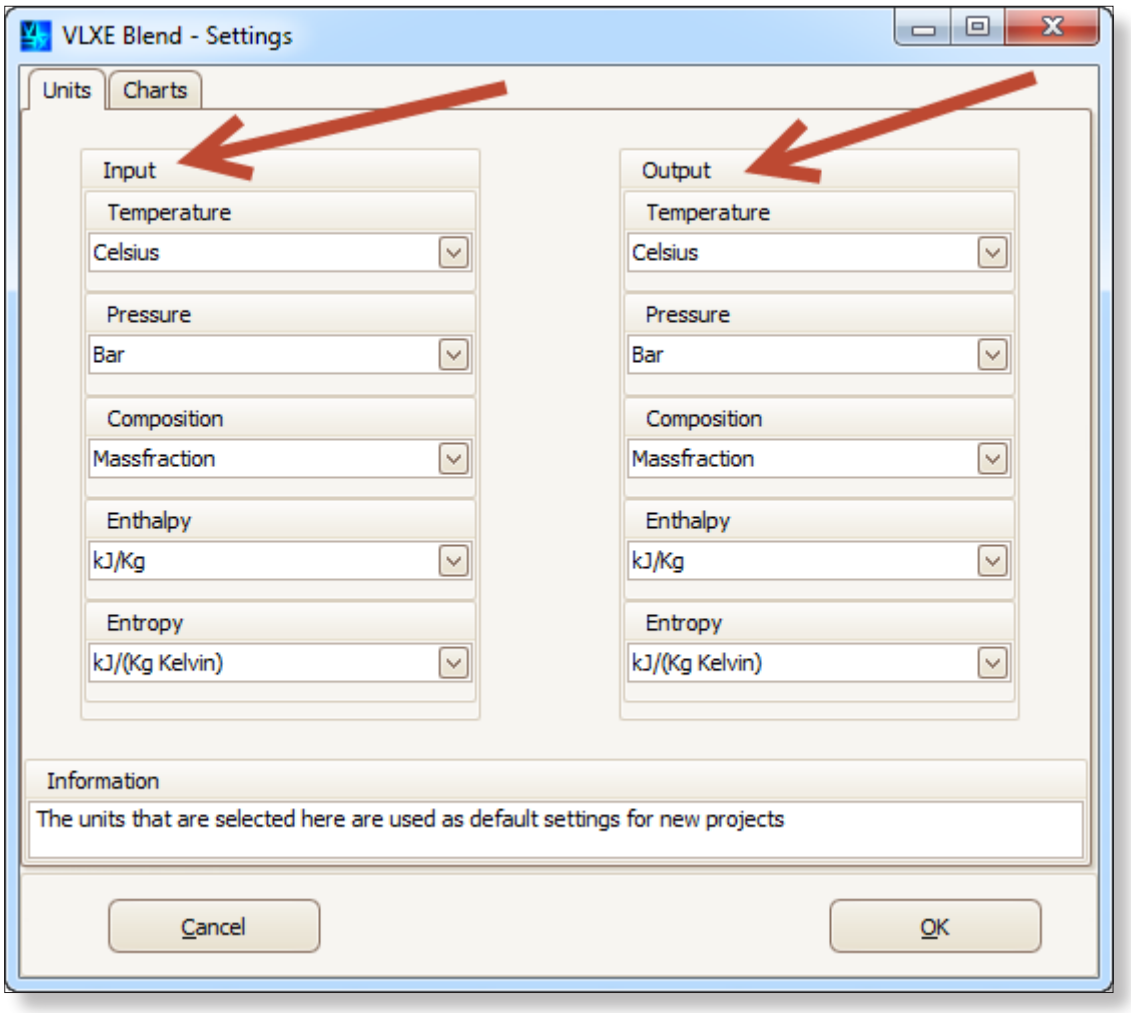


2.1.3 Standard settings

In VLXE Blend each calculation has its own unit set. This is done using a unit argument for each calculation. However, a user will often work with the same set of units, and VLXE Blend allows the user to define a standard set of units that are used by the wizards each time a new calculation is created.

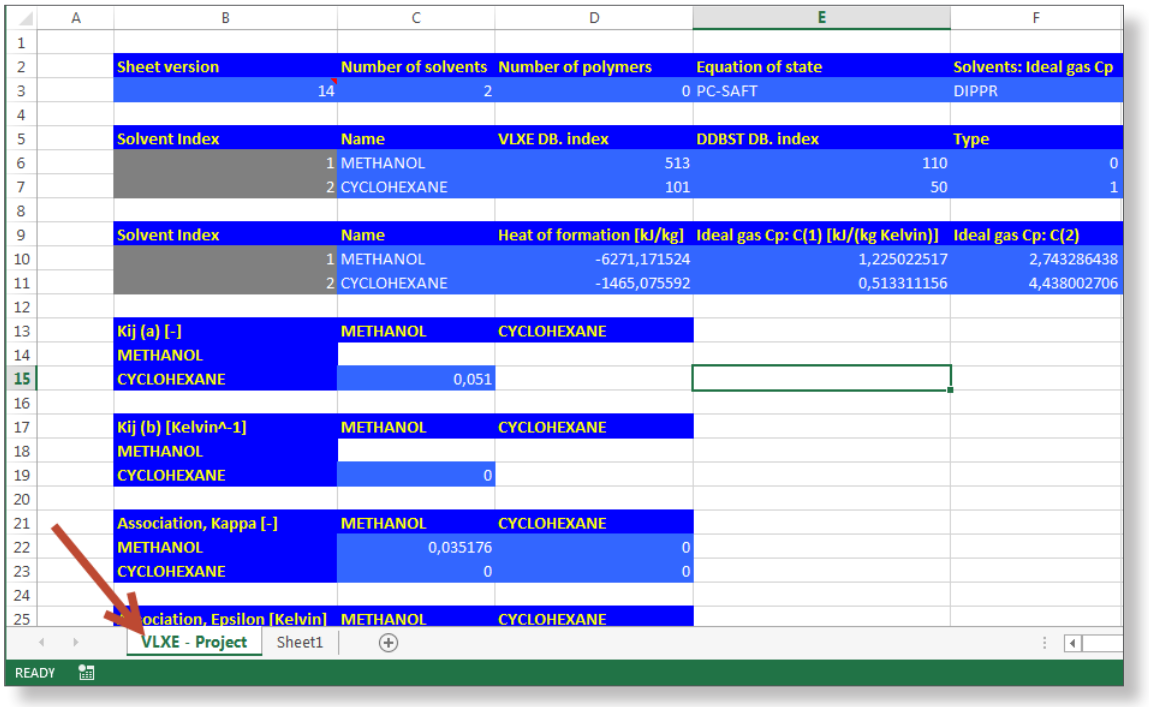
You set the default unit settings on the VLXE Blend ribbon under “Settings”.

Click on the “Standard” icon to open the settings. In the menu you can set the default in- and out-put units.



2.2 How does the databases work?

In order to run a calculation a project sheet stating the model and parameters must be provided. When creating a new project sheet the parameters are taken from the VLXE database. Once the project sheet is created any change to the database has no effect on the project sheet.



Sheet version	Number of solvents	Number of polymers	Equation of state	Solvents: Ideal gas Cp
14	2	0	PC-SAFT	DIPPR

Solvent Index	Name	VLXE DB. index	DDBST DB. index	Type
1	METHANOL	513	110	0
2	CYCLOHEXANE	101	50	1

Solvent Index	Name	Heat of formation [kJ/kg]	Ideal gas Cp: C(1) [kJ/(kg Kelvin)]	Ideal gas Cp: C(2)
1	METHANOL	-6271,171524	1,225022517	2,743286438
2	CYCLOHEXANE	-1465,075592	0,513311156	4,438002706

Kij (a) [-]	METHANOL	CYCLOHEXANE
METHANOL		
CYCLOHEXANE	0,051	

Kij (b) [Kelvin^-1]	METHANOL	CYCLOHEXANE
METHANOL		
CYCLOHEXANE	0	

Association, Kappa [-]	METHANOL	CYCLOHEXANE
METHANOL	0,035176	0
CYCLOHEXANE	0	0

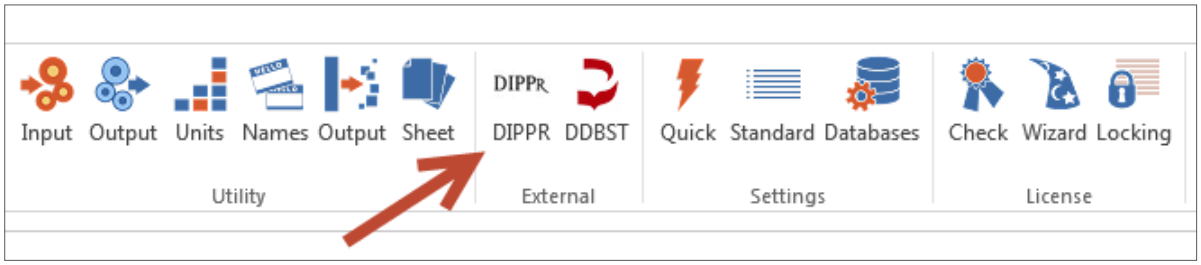
ociation, Epsilon [Kelvin]	METHANOL	CYCLOHEXANE

VLXE - Project | Sheet1 | READY

2.3 How to get properties from DIPPR using just a few clicks

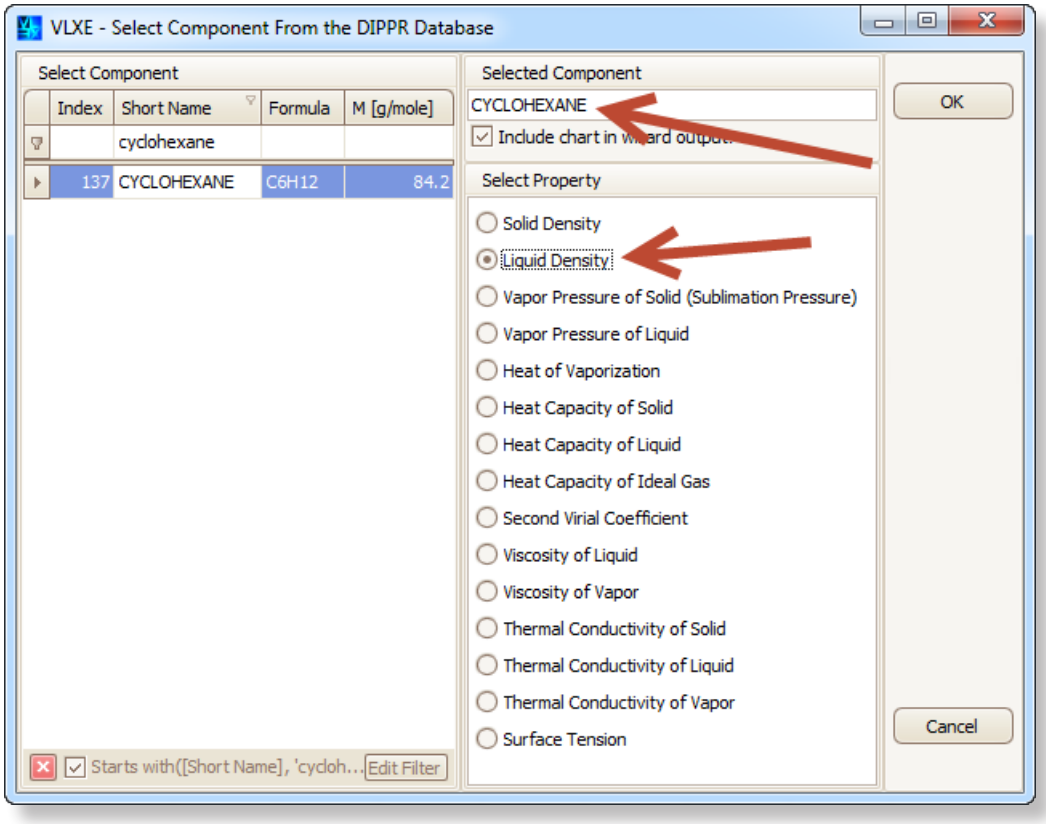
VLXE Blend makes it very easy to obtain temperature dependent properties from DIPPR.
Simply use the DIPPR wizard to make the calculation including a plot created inside Excel.

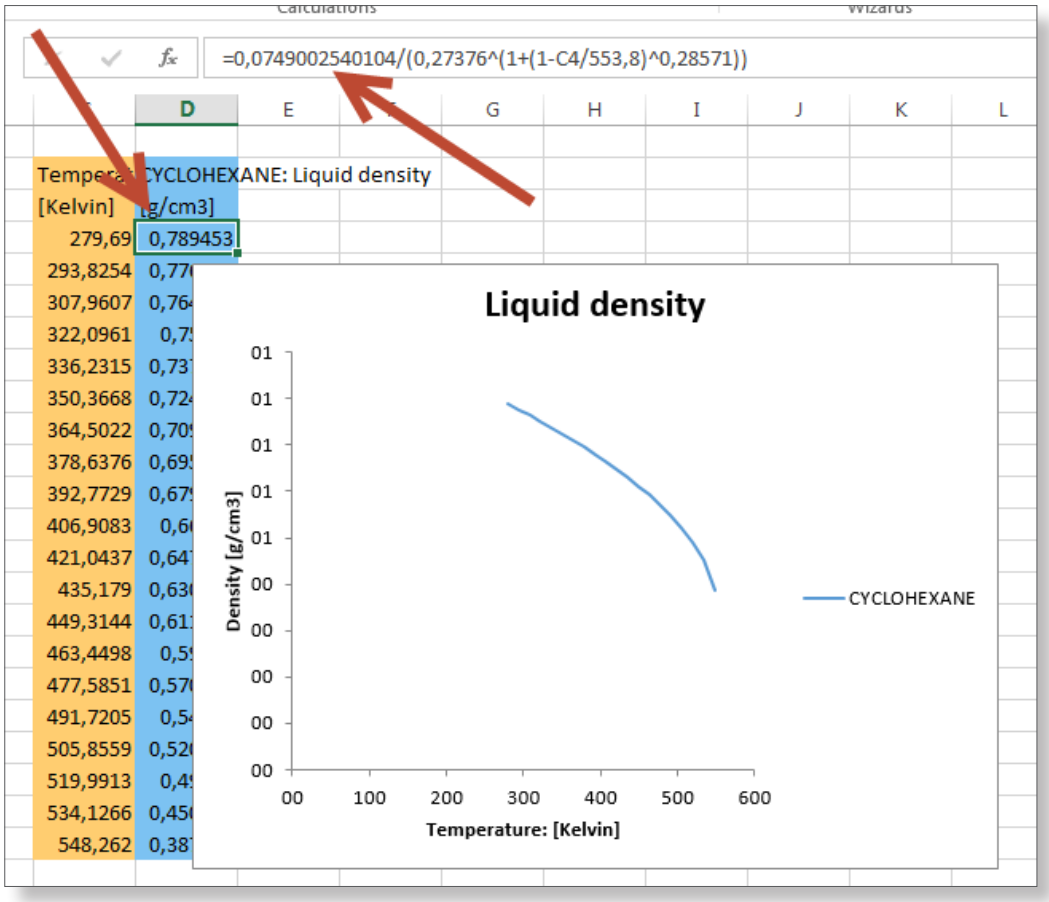
To open the wizard select “DIPPR” on the VLXE Blend ribbon.



In the DIPPR wizard that opens up first select componet and then property. The select “OK”.
Here we will use the liquid density for cycloHexane as example.

Once created, the temperature can be changed to obtain a value for the liquid density at the desired value.



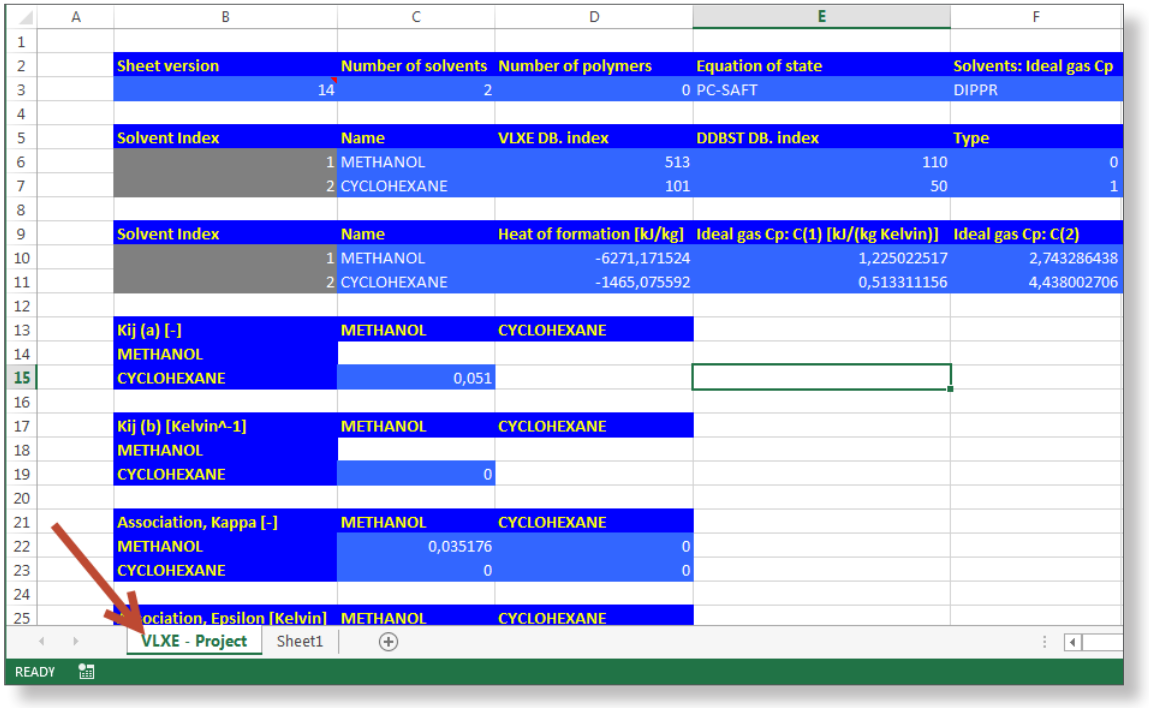


2.3.1. VLXE Project Sheet

The project sheet holds all model information. It is called before each calculation and can be edited at any time. There is no difference between a project sheet and any other Excel sheet.
Note that the sheet can be given any name.

VLXE Blend supports multi-project sheets. A function argument can be used to tell each calculation which project sheet to use.

Do not place any extra information in the project sheet. It may corrupt its reading.



	Sheet version	Number of solvents	Number of polymers	Equation of state	Solvents: Ideal gas Cp
	14	2	0	PC-SAFT	DIPPR

Solvent Index	Name	VLXE DB. index	DDBST DB. index	Type
1	METHANOL	513	110	0
2	CYCLOHEXANE	101	50	1

Solvent Index	Name	Heat of formation [kJ/kg]	Ideal gas Cp: C(1) [kJ/(kg Kelvin)]	Ideal gas Cp: C(2)
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Kij (a) [-]	METHANOL	CYCLOHEXANE
METHANOL		
CYCLOHEXANE	0,051	

Kij (b) [Kelvin^-1]	METHANOL	CYCLOHEXANE
METHANOL		
CYCLOHEXANE	0	

Association, Kappa [-]	METHANOL	CYCLOHEXANE
METHANOL	0,035176	0
CYCLOHEXANE	0	0

ociation, Epsilon [Kelvin]	METHANOL	CYCLOHEXANE

VLXE - Project | Sheet1

READY

2.3.2 How do the calculations work?

VLXE Blend performs a calculation using extra Excel functions. These functions work just like any other function in Excel.

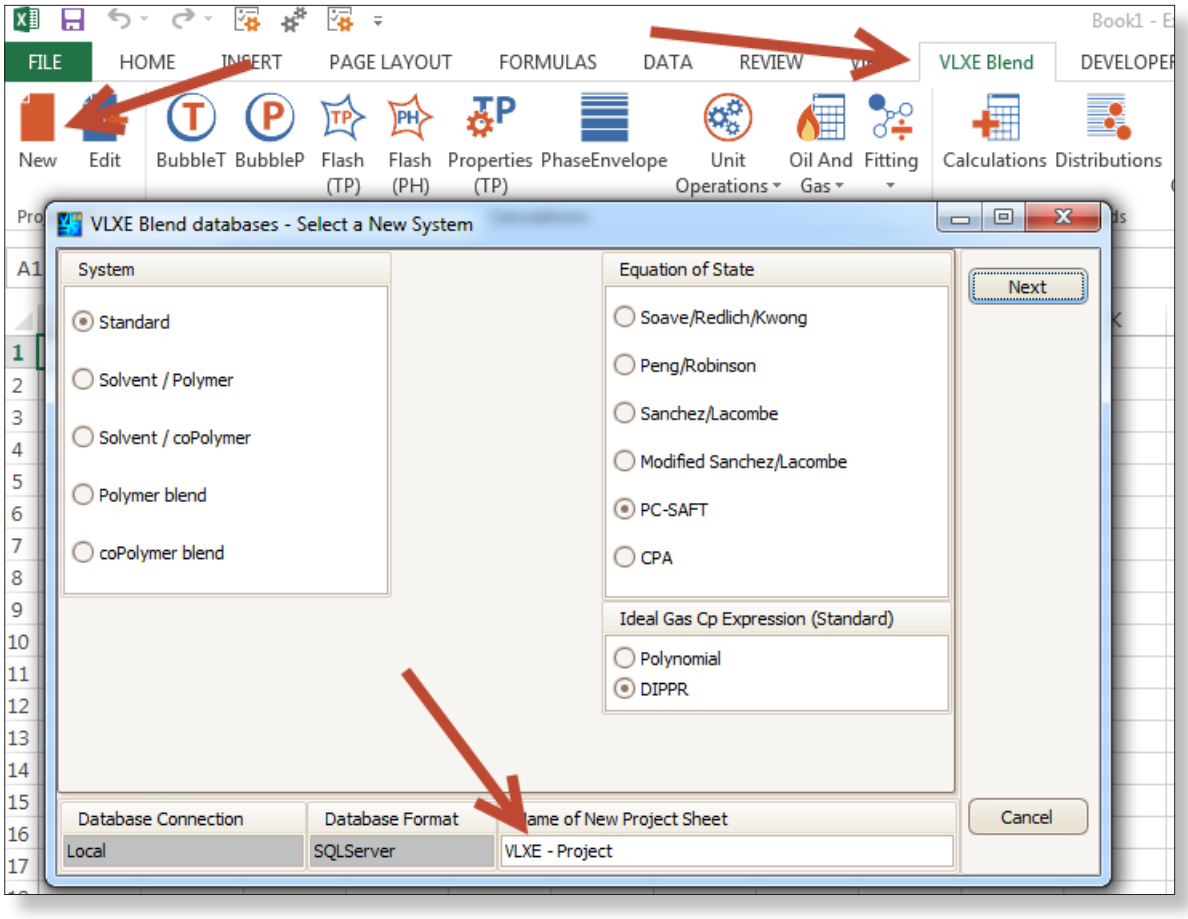
Each calculation needs 2 sets of input:

- System information: Model, parameters etc.
- User information: Temperature, pressure, feed etc.

When a calculation is run, the project sheet is read. Then the arguments to the function are read and the calculation is performed.

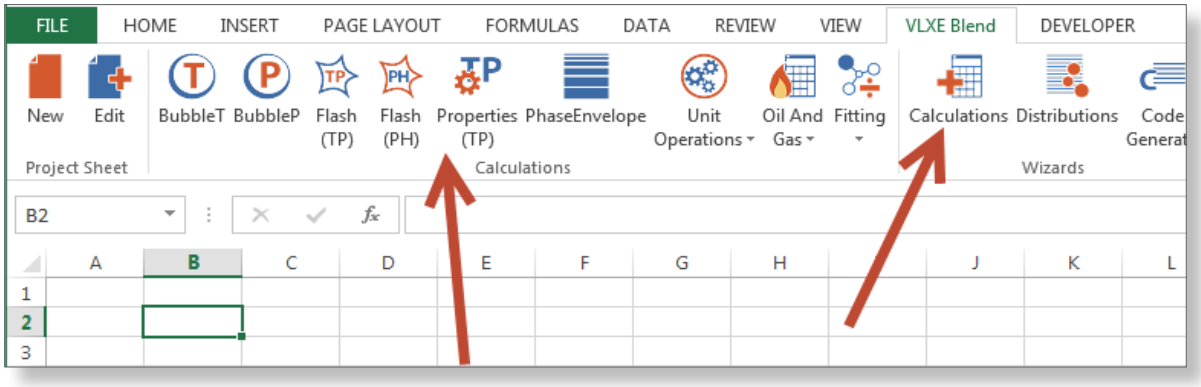
2.4 New from database

This opens a wizard that helps the user define a new project sheet.
The parameters are taken from the database and can be edited at any time. Subsequent changes to the database have no effect on the project sheet. A project sheet can be created by hand, but it is far easier to use the wizard.



2.5 Standard Wizards

Thermodynamic calculations may require a large range of input and output values, to aid the user a number of wizards are provided. A full wizard covering all calculations can be opened plus the most commonly used calculations are placed directly on the VLXE Blend Ribbon (select the components to include) and output properties.



2.6 Common function arguments

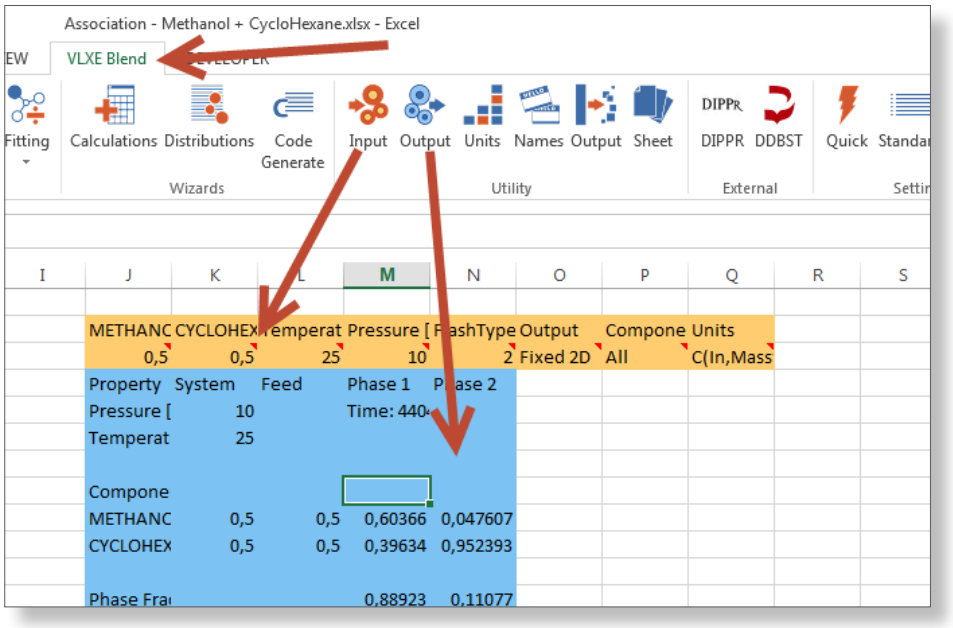
A few arguments are used in all the VLXE Blend functions. They provide you with full flexibility.

They are:
Output - Lets you select the desired output from a calculation.
Components - You can select all or part of the components in the project sheet.
Units - Defines the units used in this calculation.
Distribution - Lets you override the polymer distribution given in the project sheet.
BlockMass fraction - Used for coPolymer only. Lets you override the blockmass fraction given in the project sheet.
AdvVLXE - used internally by VLXE.
AdvUser - Provided for the users´ convience. Can be used, for example, to trigger the function to recalculate, if the content of the referenced cell is changed.

2.7 Input and Output Color Scheme

In order to keep the Excel sheet organized, VLXE Blend uses a color scheme. Orange color represents input to the calculation and blue color represents output.

If a calculation is created using the wizard, the colorscheme is applied automatically. If you create a calculation by hand or change a existing one, the colors can be set using the buttons provided in the VLXE Blend ribbon.

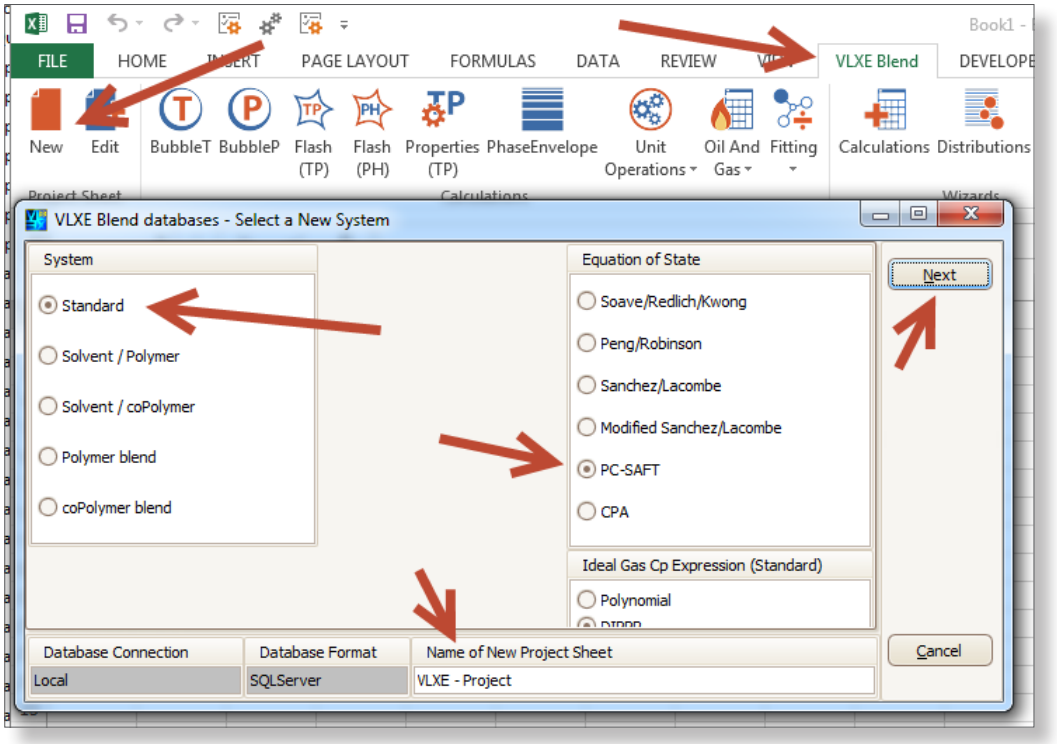


3) Basic Features

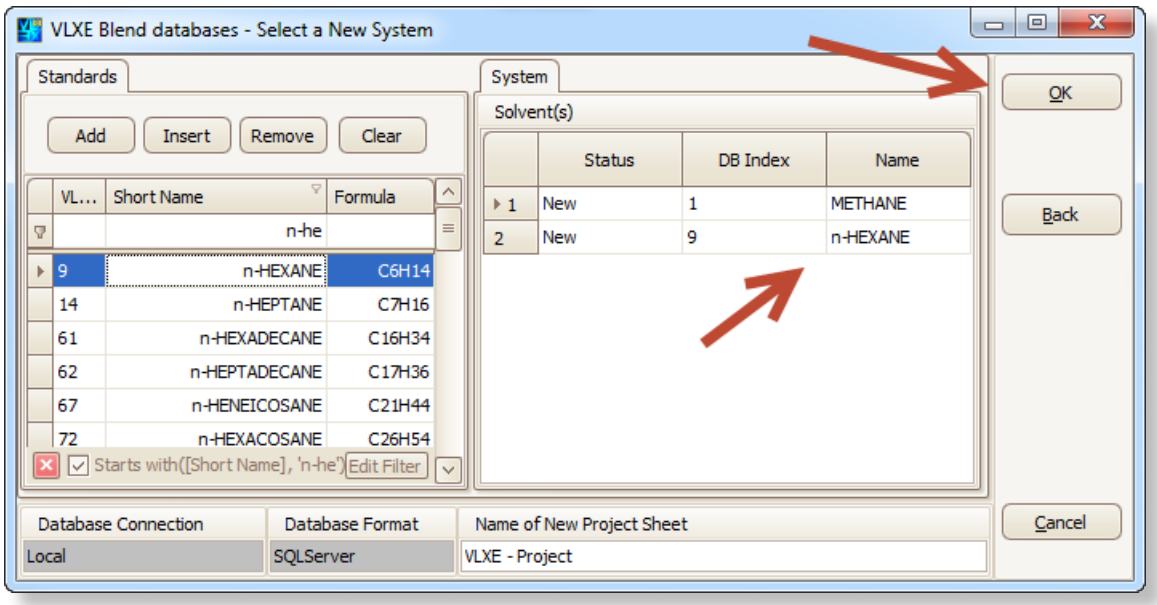
3.1 How to Create a New Project

1. Open Excel, select “New” on the VLXE Blend ribbon.

2. In the window that opens select “System” on the left side and “Model” on the right side. In the lower right side you can change the name of the project sheet, if so desired. Note also how database information is given on the lower left side

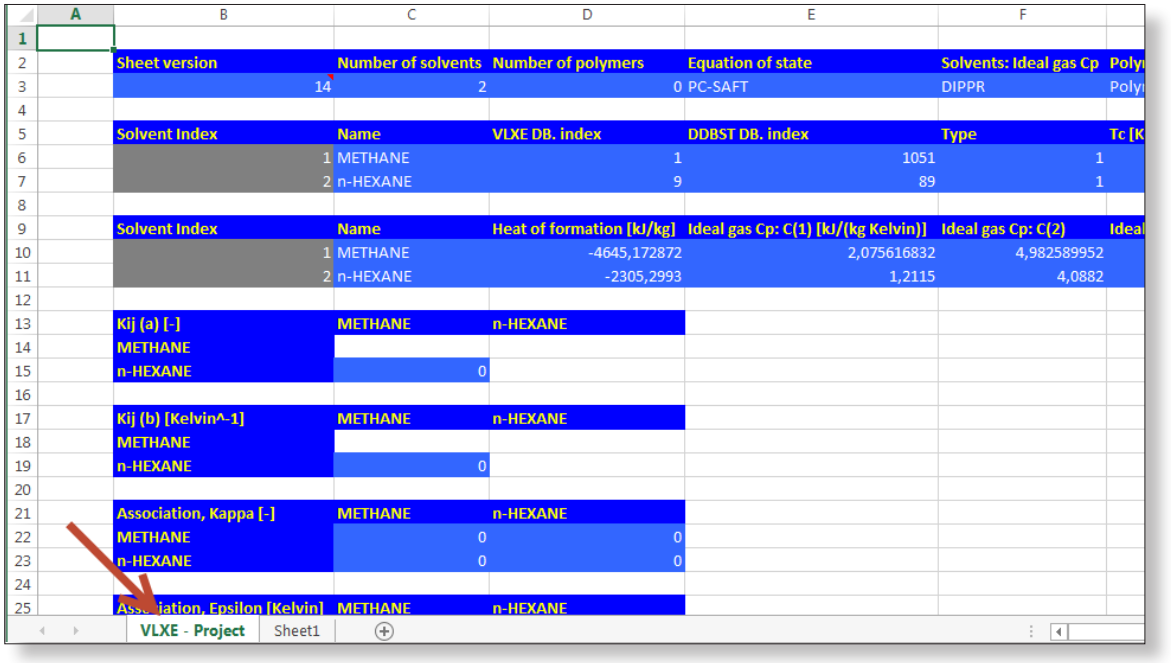


3. Click “Next” and add solvents from the data bank to define the system.



4. Click “OK”. A new project sheet is now created.

Note how the model and parameters are included in the sheet. The sheet can be changed at any time, if needed.



	A	B	C	D	E	F
1						
2		Sheet version	Number of solvents	Number of polymers	Equation of state	Solvents: Ideal gas Cp
3		14	2	0	PC-SAFT	DIPPR
4						
5		Solvent Index	Name	VLXE DB. index	DDBST DB. index	Type
6		1	METHANE	1	1051	1
7		2	n-HEXANE	9	89	1
8						
9		Solvent Index	Name	Heat of formation [kJ/kg]	Ideal gas Cp: C(1) [kJ/(kg Kelvin)]	Ideal gas Cp: C(2)
10		1	METHANE	-4645,172872	2,075616832	4,982589952
11		2	n-HEXANE	-2305,2993	1,2115	4,0882
12						
13		Kij (a) [-]	METHANE	n-HEXANE		
14		METHANE				
15		n-HEXANE	0			
16						
17		Kij (b) [Kelvin^-1]	METHANE	n-HEXANE		
18		METHANE				
19		n-HEXANE	0			
20						
21		Association, Kappa [-]	METHANE	n-HEXANE		
22		METHANE	0	0		
23		n-HEXANE	0	0		
24						
25		Association, Epsilon [Kelvin]	METHANE	n-HEXANE		

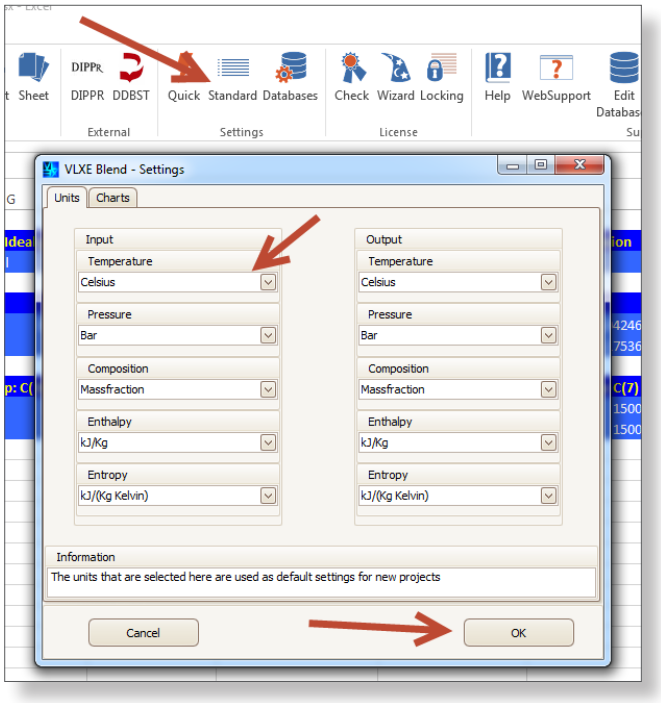
VLXE - Project | Sheet1

3.2 Edit the Default Settings

The default settings in VLXE Blend include unit settings. Each calculation has its own set of units, but the settings here are used as default values when creating a new calculation.

To change the default settings follow these steps:

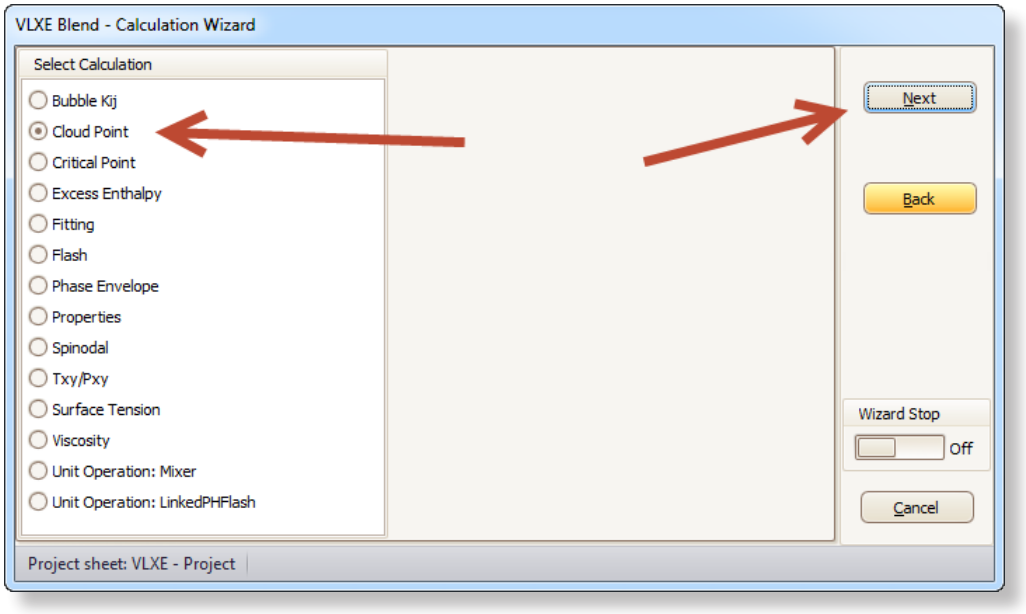
1. On the VLXE Blend ribbon, select “Standard Settings” click “Settings” to open the standard settings menu. Click on “Units”, here you see the default settings for all the units.



3.3 Creating a new calculation: Cloud point example

All calculations in VLXE Blend are created using the same steps as in the wizard provided. The steps below will create a cloud point calculation using the project sheet just made.

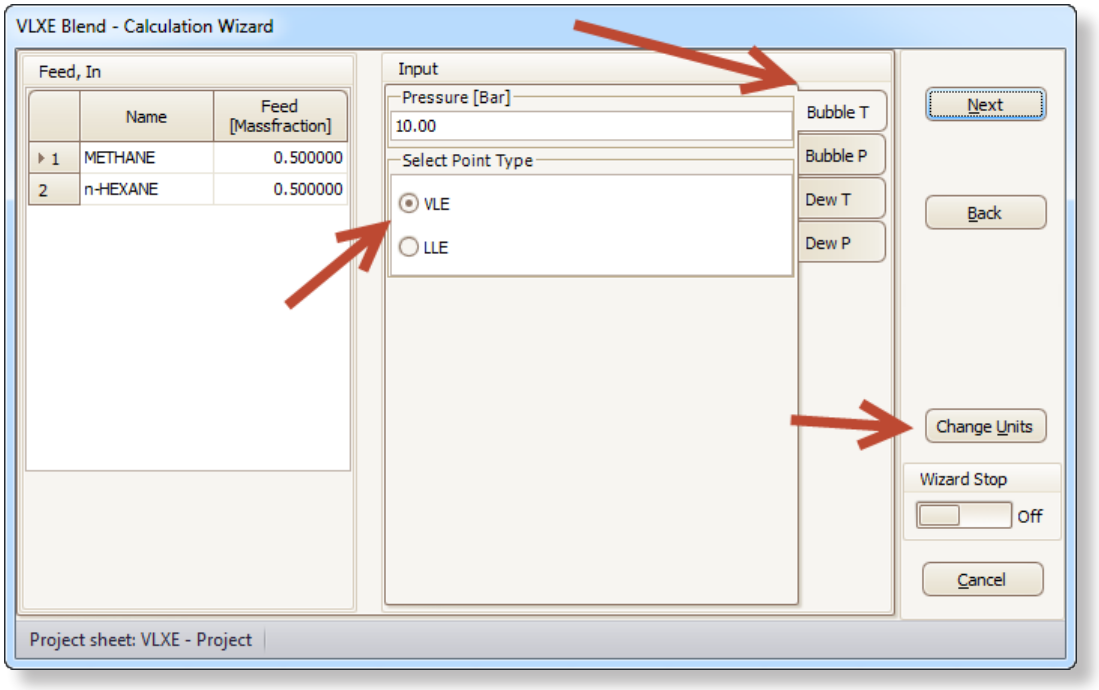
1: Select “Calculations” under “Wizards” in the “VLXE Blend” menu.
2: Leave the component part unchanged and select “Next”.
3: Select “Cloud Point” on the right side and select “Next”.
4: Select “Cloud P” as type and leave the other input unchanged. Note that this can easly be changed once the wizard ihas finished.
5: Click on “Units” to check that they are as required. Now click “Next”.



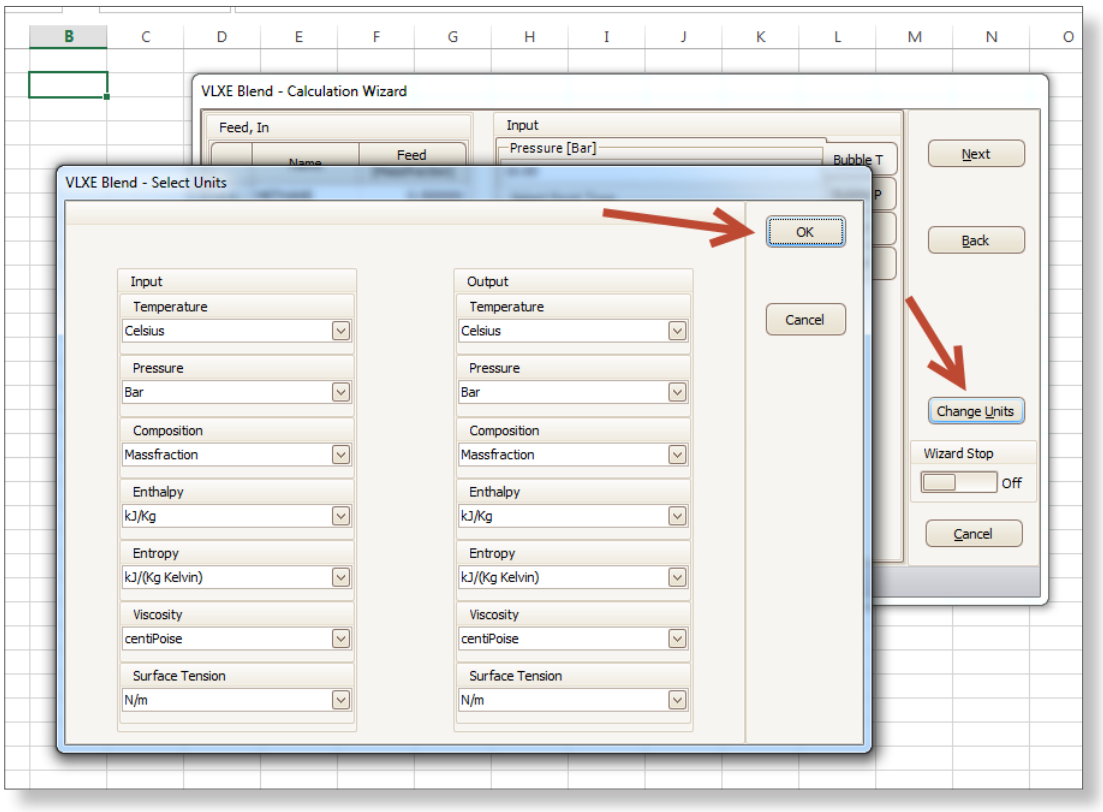
6. By clicking “Next” there are two ways of calculating a cloud point: Cloud temperature and cloud pressure.

Select: Bubble T.

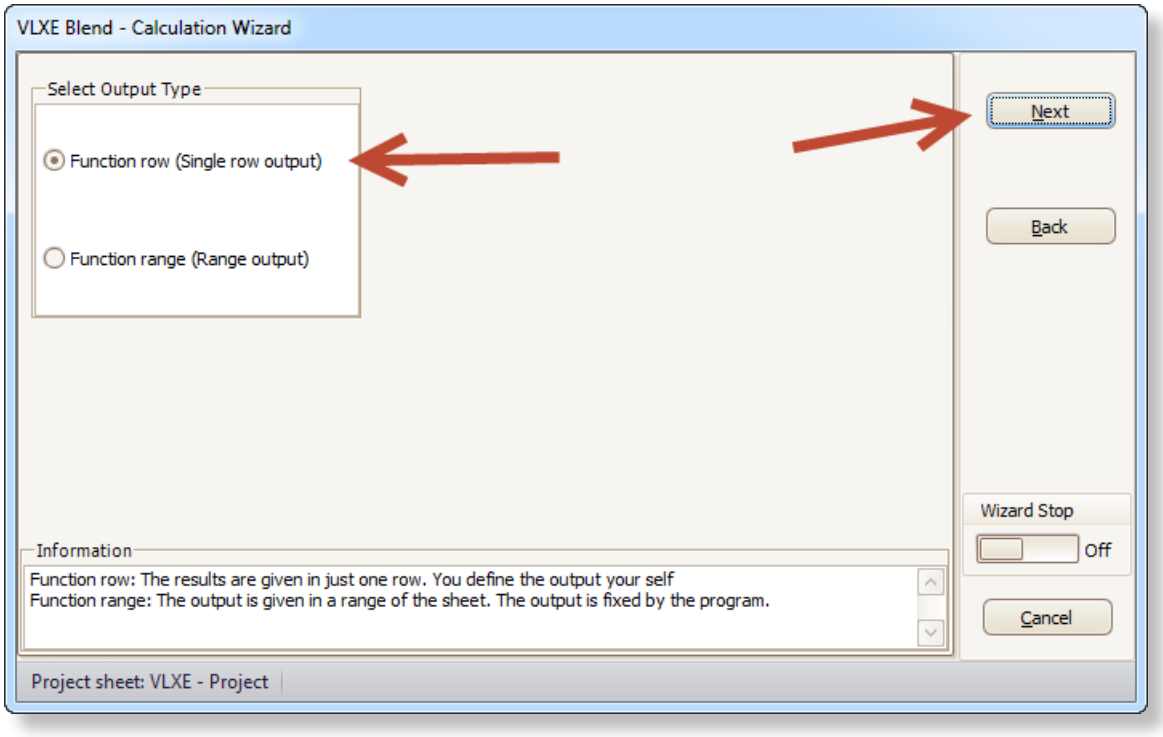
Note that in VLXE Blend a cloud and bubble point is the same.



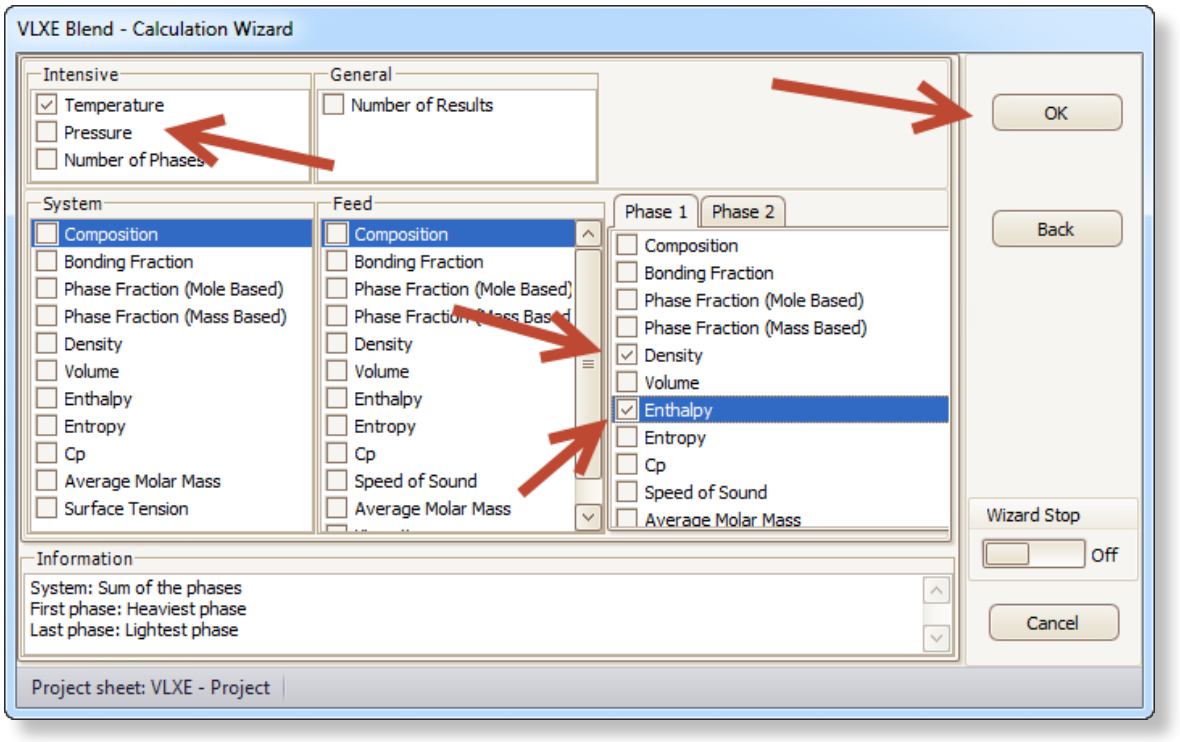
7. Units can be changed by clicking on “Change Units”. For this example, change the composition into mole fraction for input stream and then click “OK”.



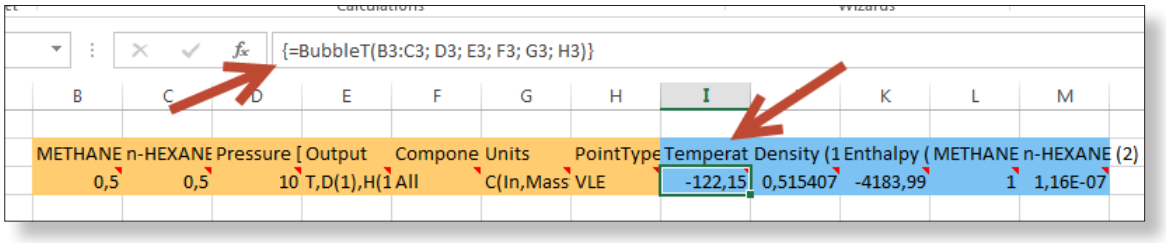
8. At this step there are two options i.e. either output type is selected as a function row - single row output, or you can request the function range - range output. First the results for function row - single row output will be shown.



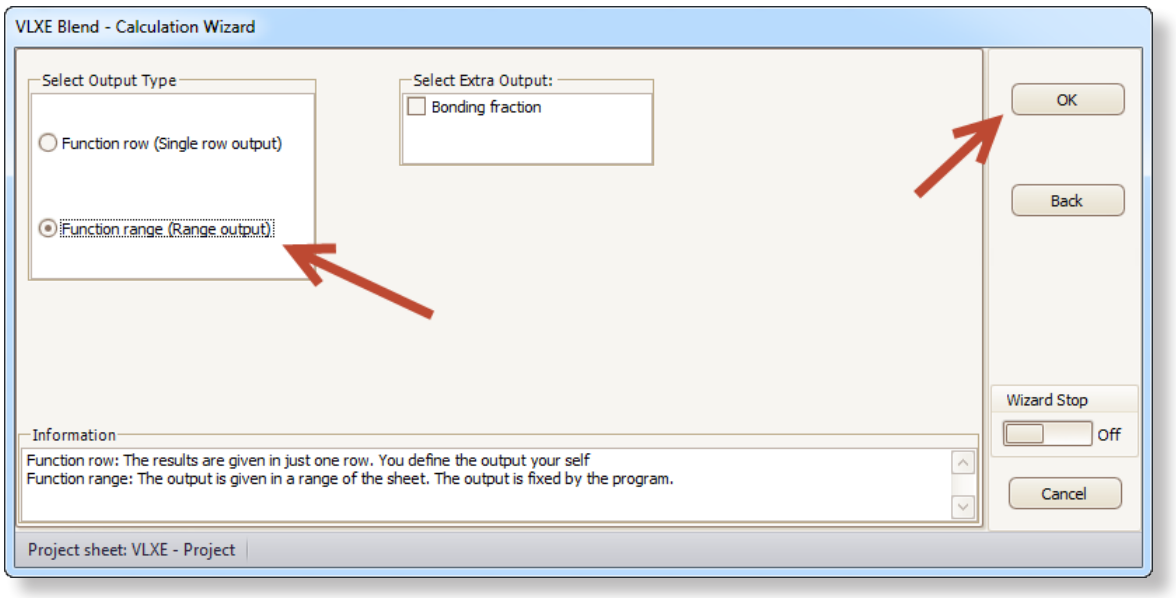
9. Click “Next” and following calculation wizard will appear.



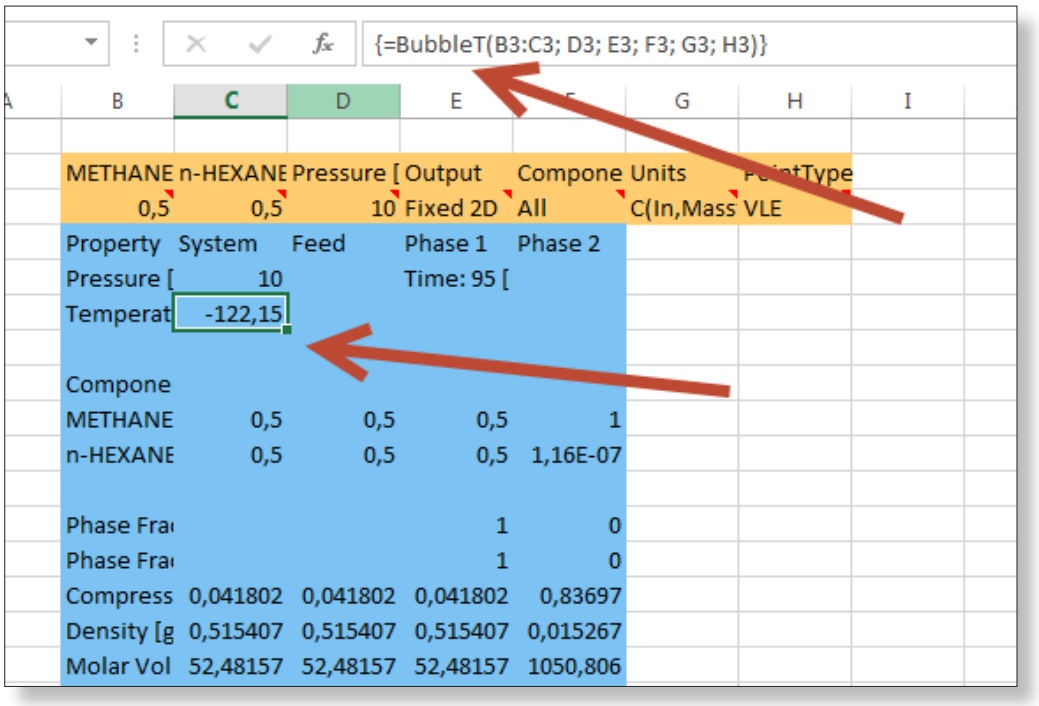
10. Click “OK” and the corresponding results are shown in the form of single row output.



11. To see the result from function range - range output, go to step 8 and click on “Function range (Range output)”.



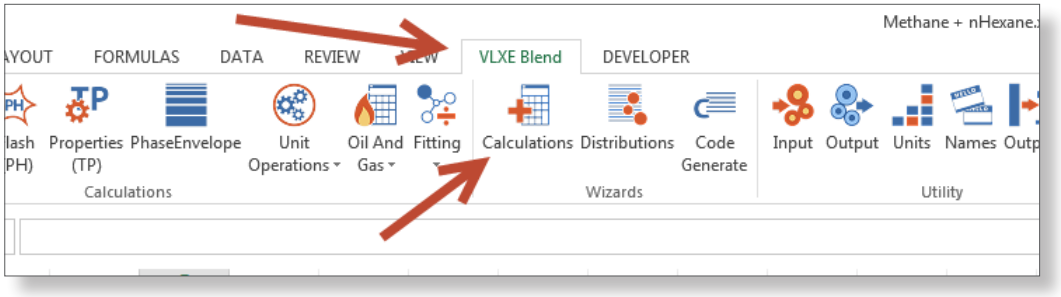
12. Click on “OK” and the result will be displayed in the Excel sheet.



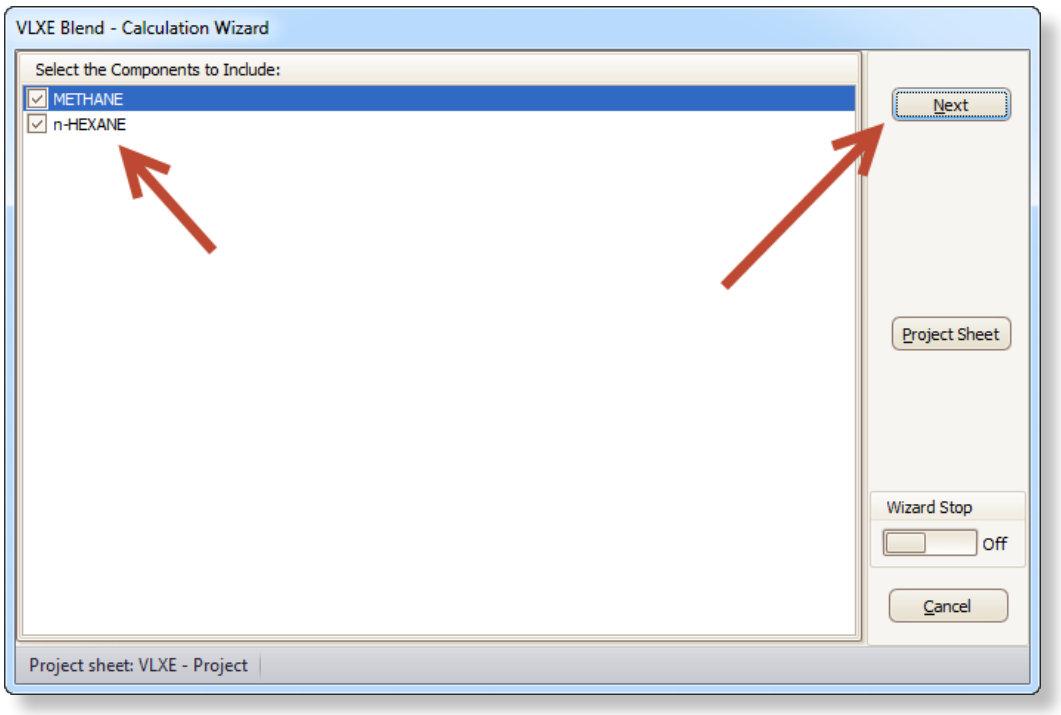
3.4 How to Perform Phase Envelope Calculations

The steps below will create a phase envelope calculation. We will use the wizard so all the work in setting up the sheet is done automatically.

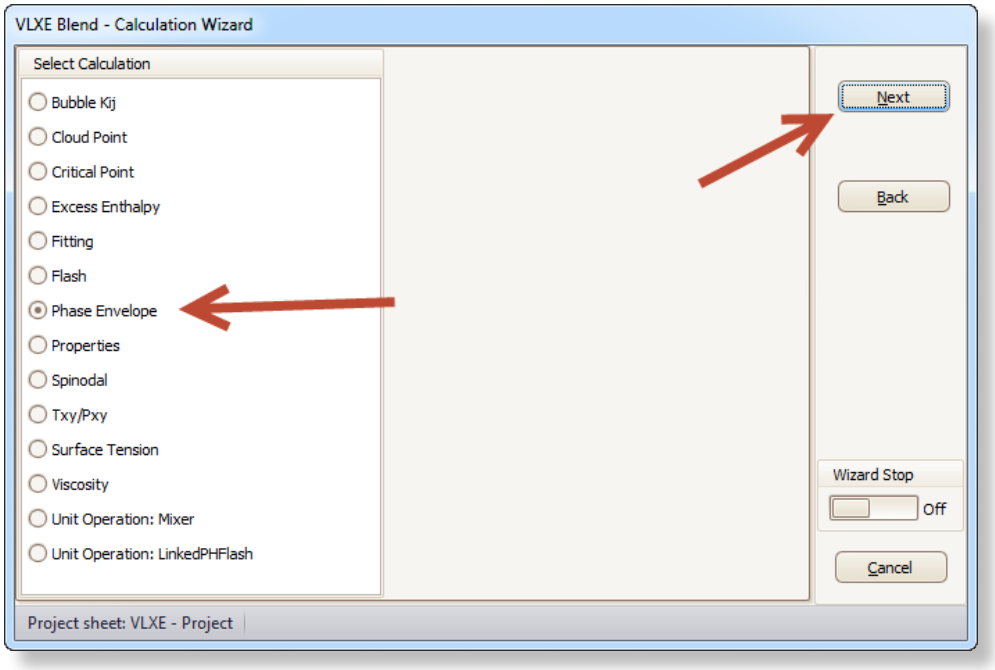
1. Click on the next Excel sheet and click on the cell where the calculations should start. Open the calculation wizard and click “Next”.



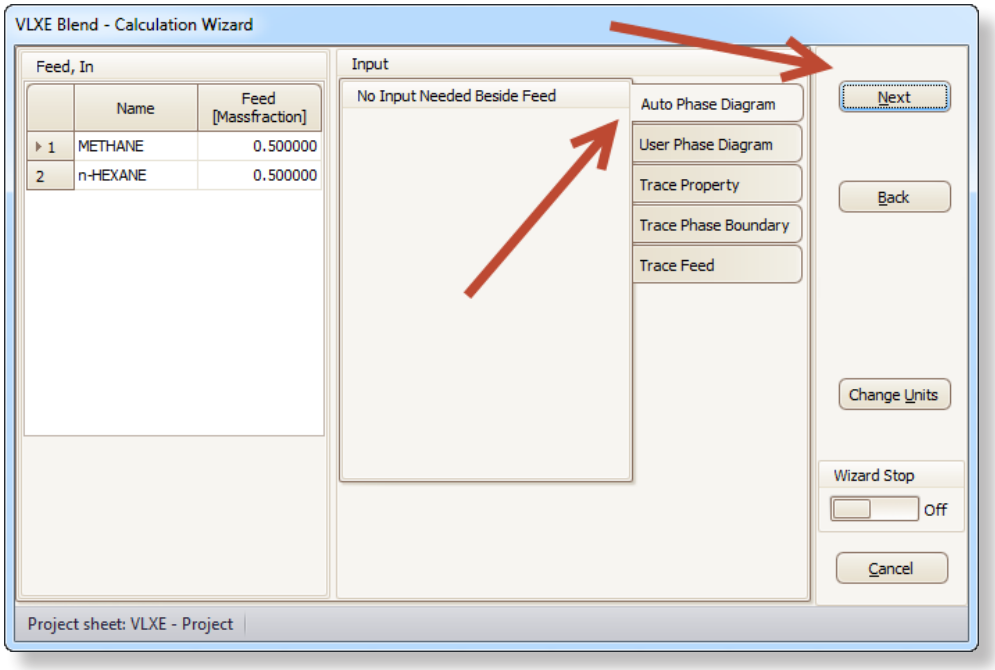
2. By clicking on “Calculations” the selected components appears.
For this case both methane and n-hexane can be seen.



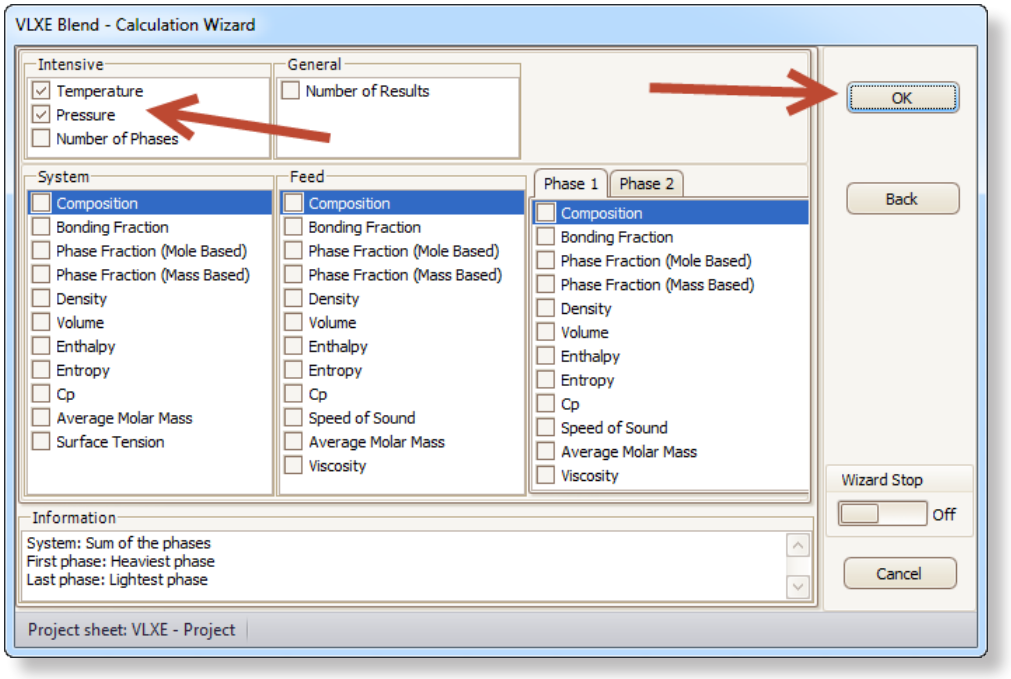
3. Click “Next” and select the property (i.e. Phase envelope)



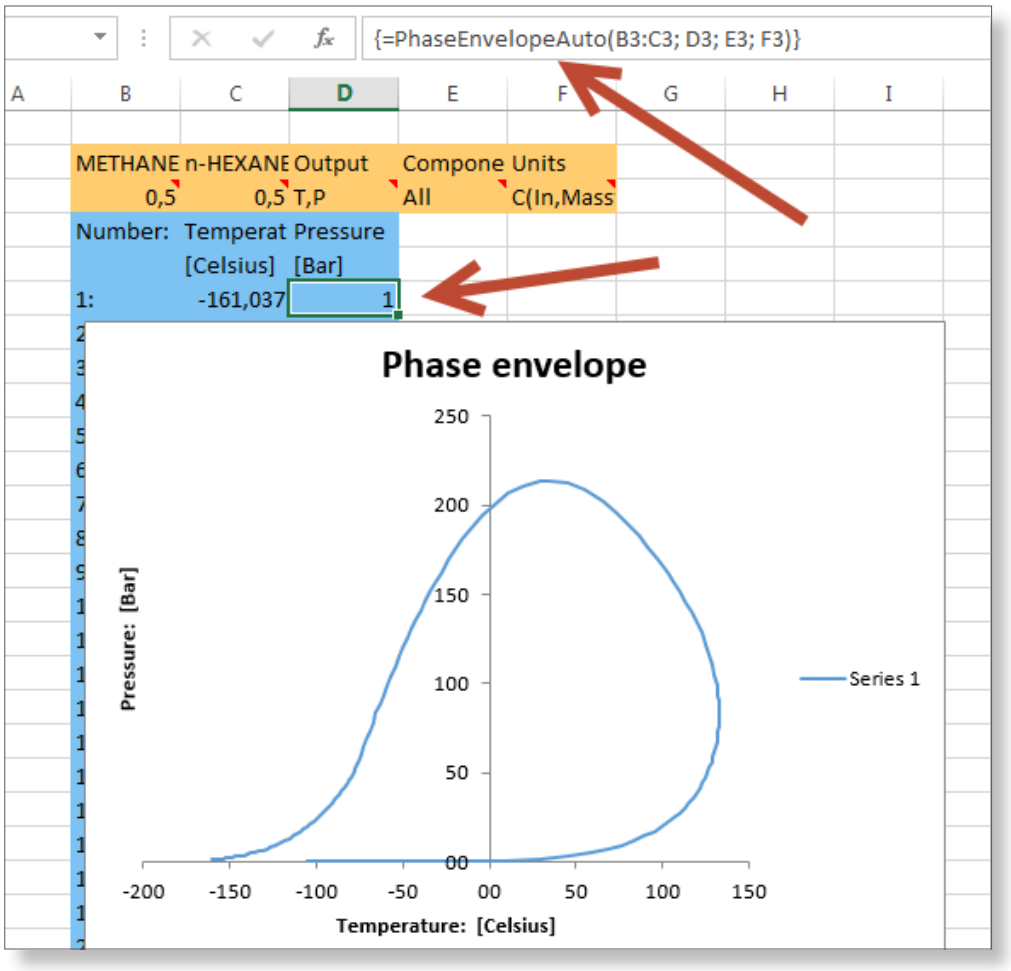
4. By clicking “Next”, the calculation wizard appears and displays some more functions like: Auto Phase Diagram, User Phase Diagram etc. For this example select “Auto Phase Diagram”.



6. Click “Next” and define the output.



7. Click “OK” and the desired results are shown in the Excel sheet. Note: The wizard also creates a chart.



3.5 How to Change the Units Used in the Calculations

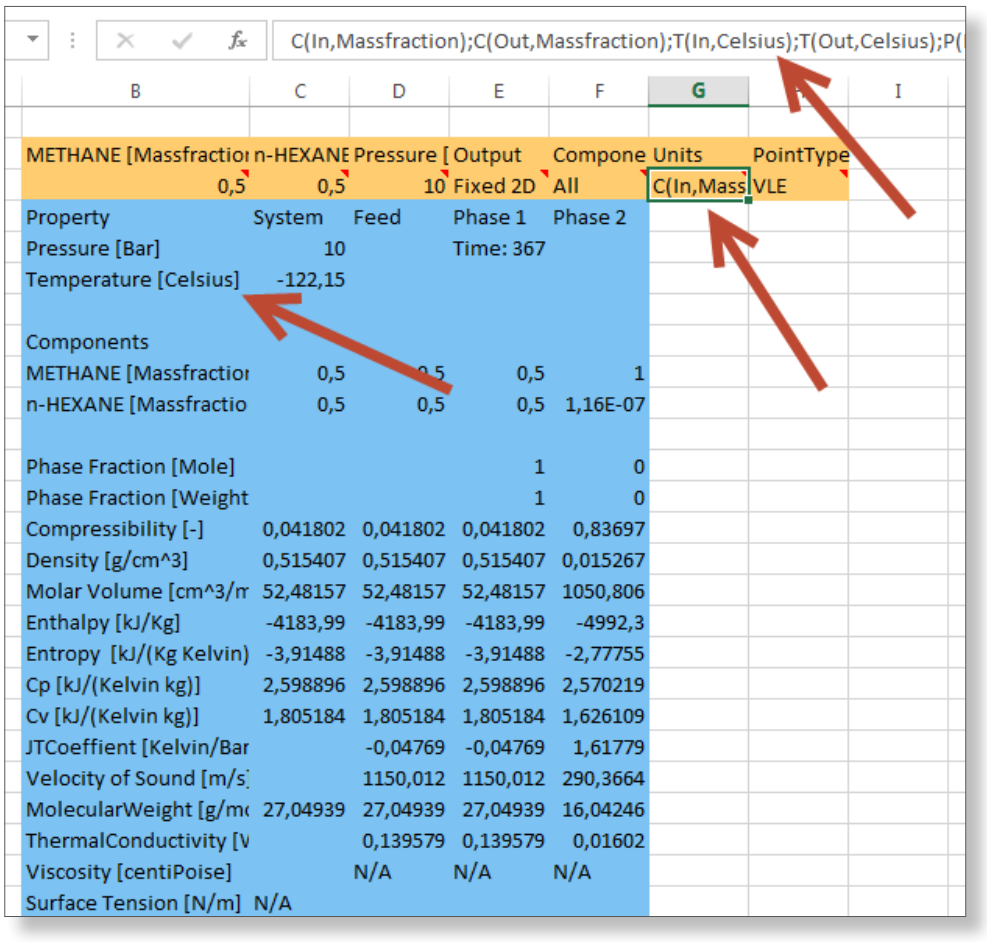
There are two ways of changing the units:
1. Manually
2. Calculation wizards

3.5.1 Manually

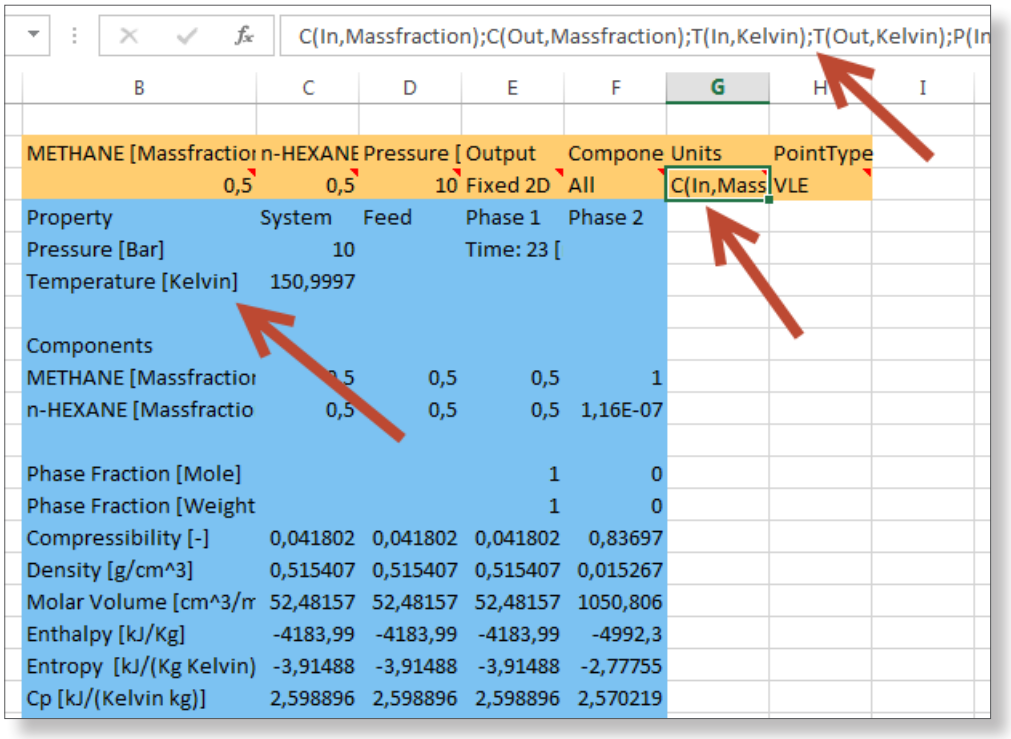
Once an output is obtained, for example, a cloud point. The units can be changed by following these steps. (As an example, temperature units are to be changed from Celsius to Kelvin).

1. Click on the units cell, input and output units are given in Celsius. To change from Celsius to Kelvin, simply type Kelvin in place of Celsius.

Note: It is case sensitive, so the first letter should be a capital and with no spelling mistakes.



The above figure shows temperature in Celsius whereas the figure shown below shows that temperature changed into Kelvin.

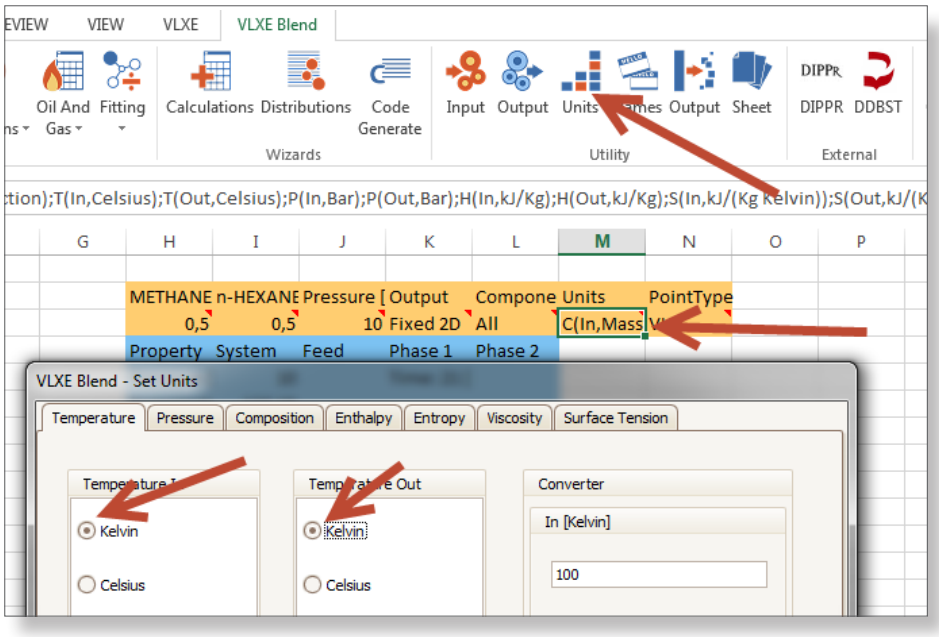


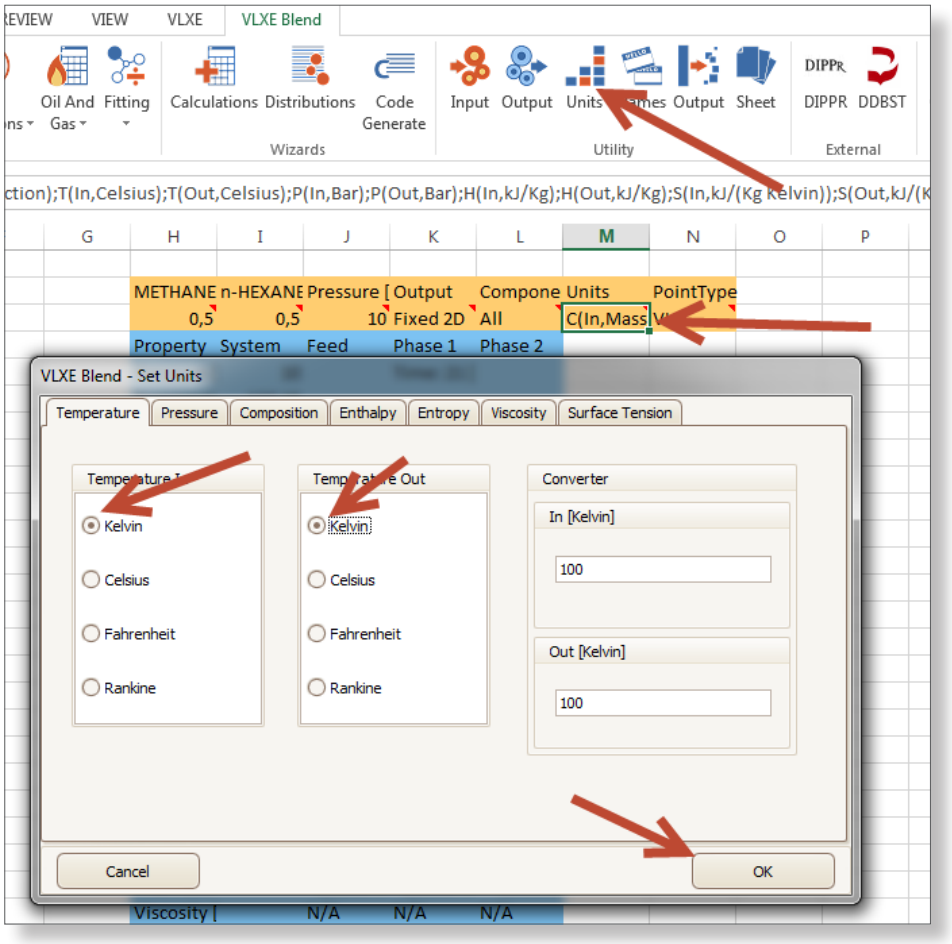
Warning: Input units labels are not updated.

3.5.2 Calculation Wizard

Units can also be changed using the Units wizard. This is a simpler process since spelling and format will all-ways be correct.

It involves the following steps:
Select the cell with a unit that needs to be changed. Click on “Units” under “Utility”. In the wizard window change temperature to “Kelvin” and click “OK”.
The units are now changed.



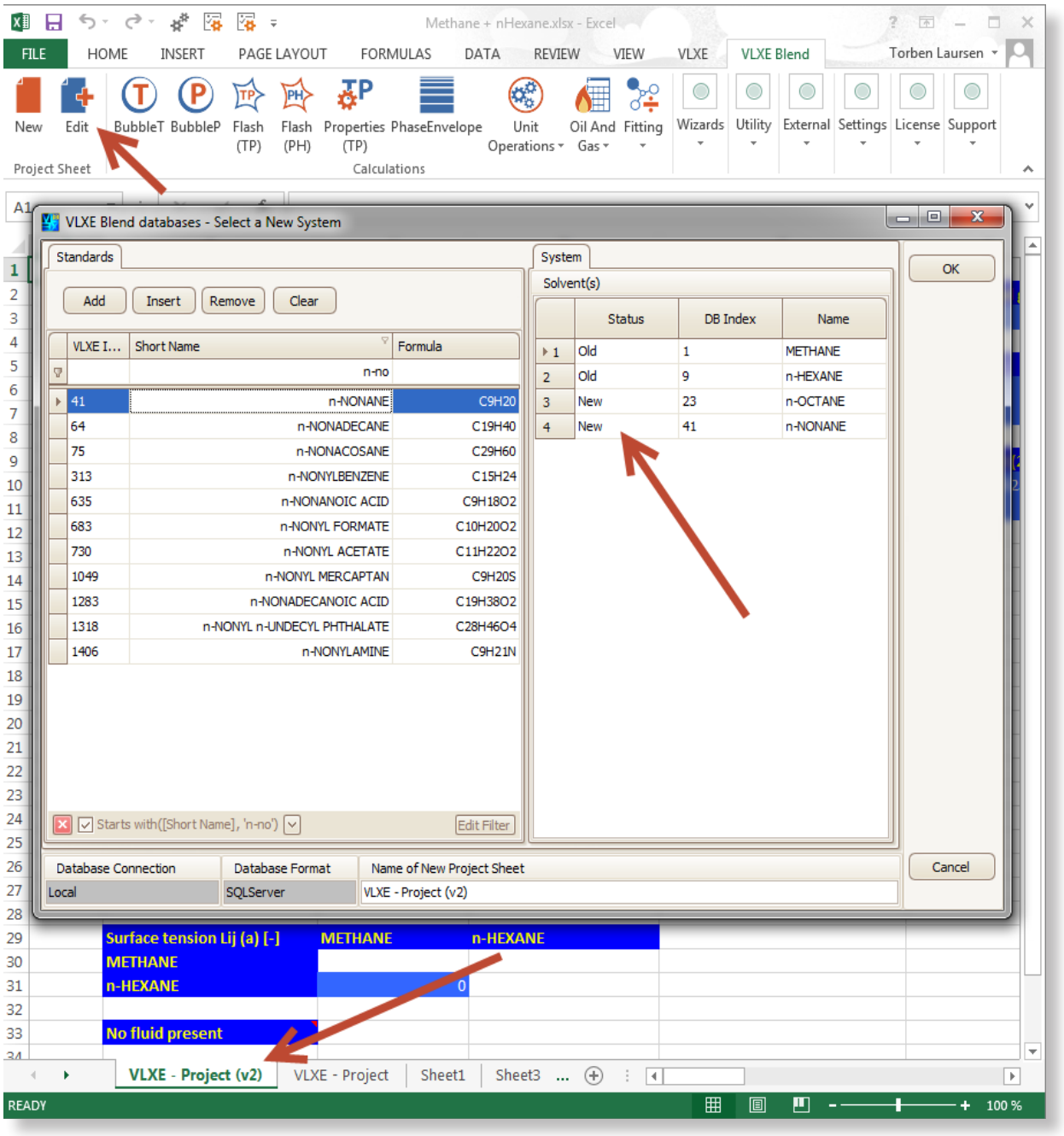


3.6 Change component list in a project sheet

The component list in a existing project sheet can be changed. This is often done by taking a copy of an existing sheet, renaming it and then adding or removing components using the VLXE Blend database.
It is possible to perform this editing by hand, but it is far better to use the wizard.

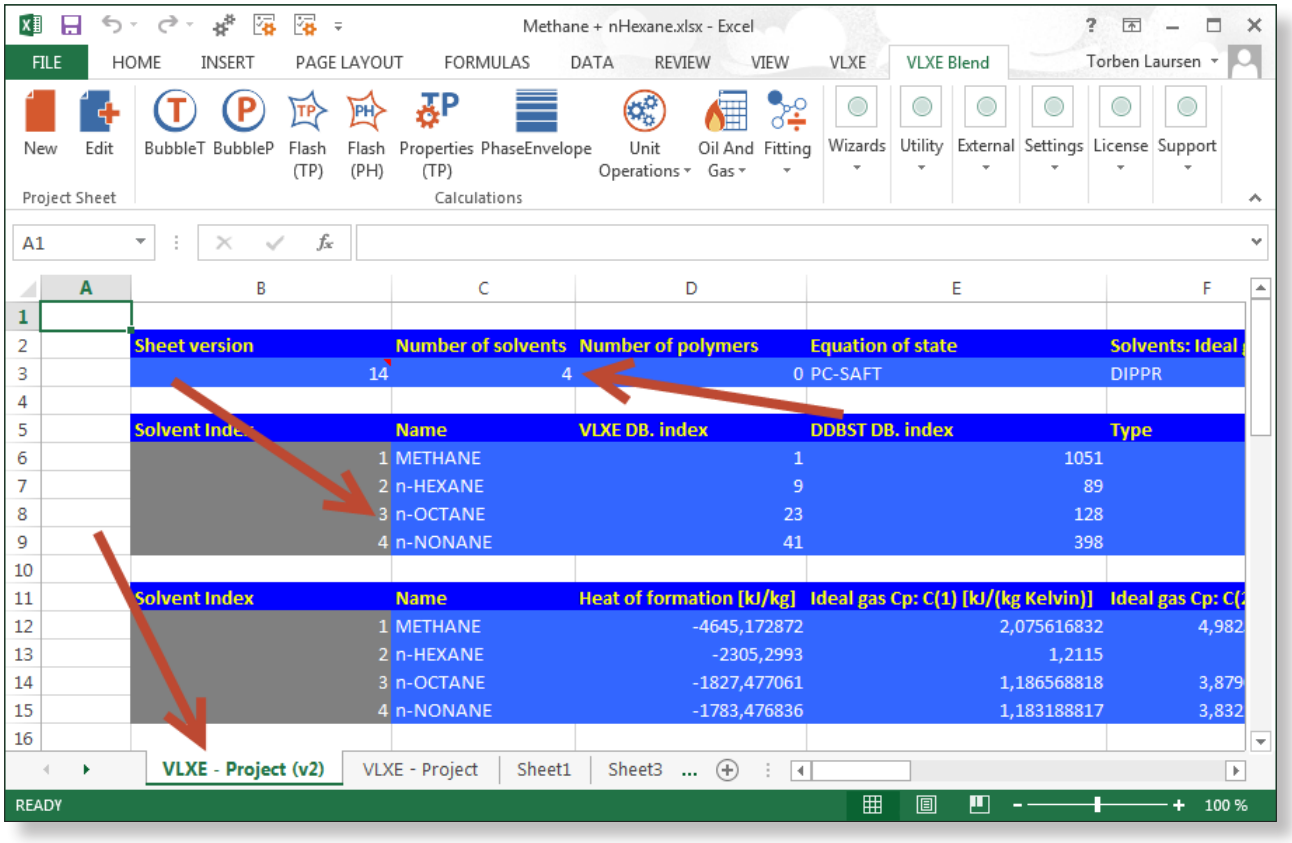
As an example, we will take the project sheet from before and add two more components from the database. In the Excel file with Methane + n-Hexane, make a copy of the project sheet and rename it to “Project Sheet (v2)”.

Then, select the sheet and click on “Edit”. In the new window select “n-Octane” and “n-Nonane” and add them to the solvent list. Note how they have “New” under “Status”.



Click on “OK” to accept the changes and then “Yes” to overwrite the existing project sheet.

The existing project sheet is now overwritten by the new Mixture which now includes the 2 new components.



3.7 Working with multi-project sheets

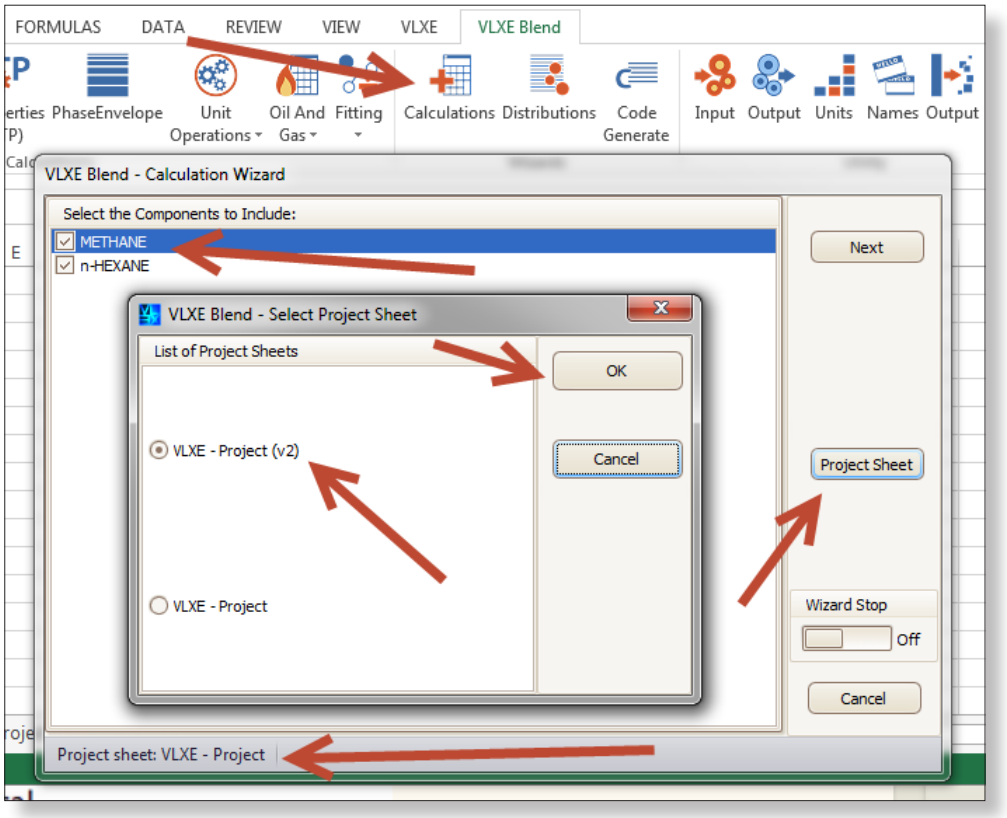
VLXE Blend supports any number of project sheets. This is done using the “ProjectSheet” argument. This is a optional argument, so if left blank, it will use the project sheet with the default name: “VLXE - Project”. Otherwise it will use the provided project sheet.

As a example we will use the file just created, it holds 2 project sheets, and create a new flash calculation.

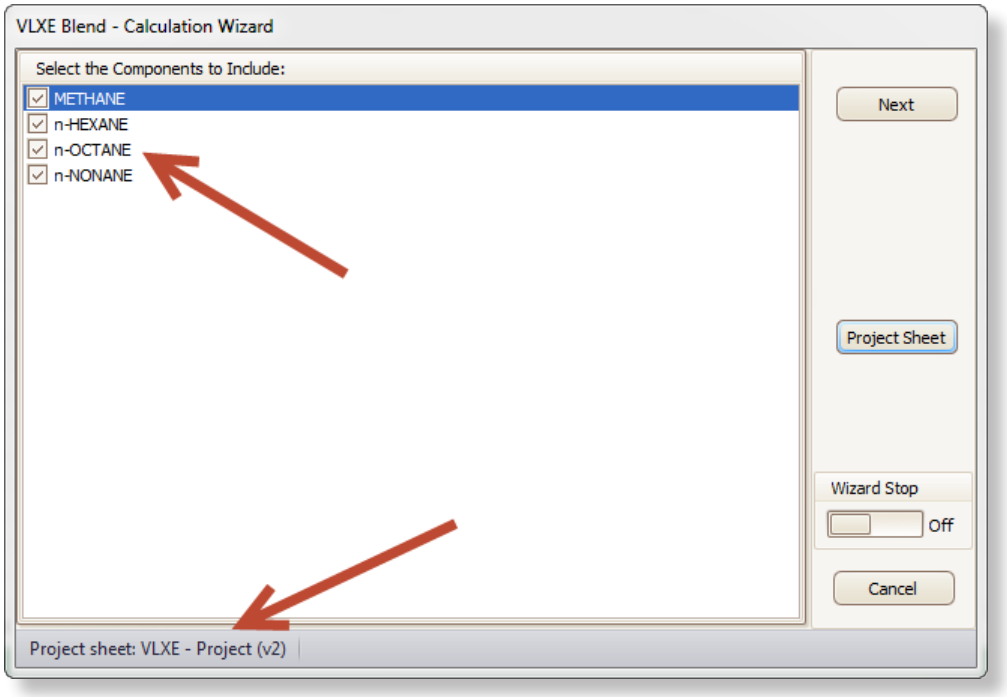
Open the Excel file and go to a blank sheet.

3.7.1 Using the calculation wizard

Open the Excel file and go to a blank sheet. Select “Calculations” on the VLXE Ribbon. VLXE Blend will remember the last project sheet used and use that as default. So now select “Project Sheet” on the right side to change it.

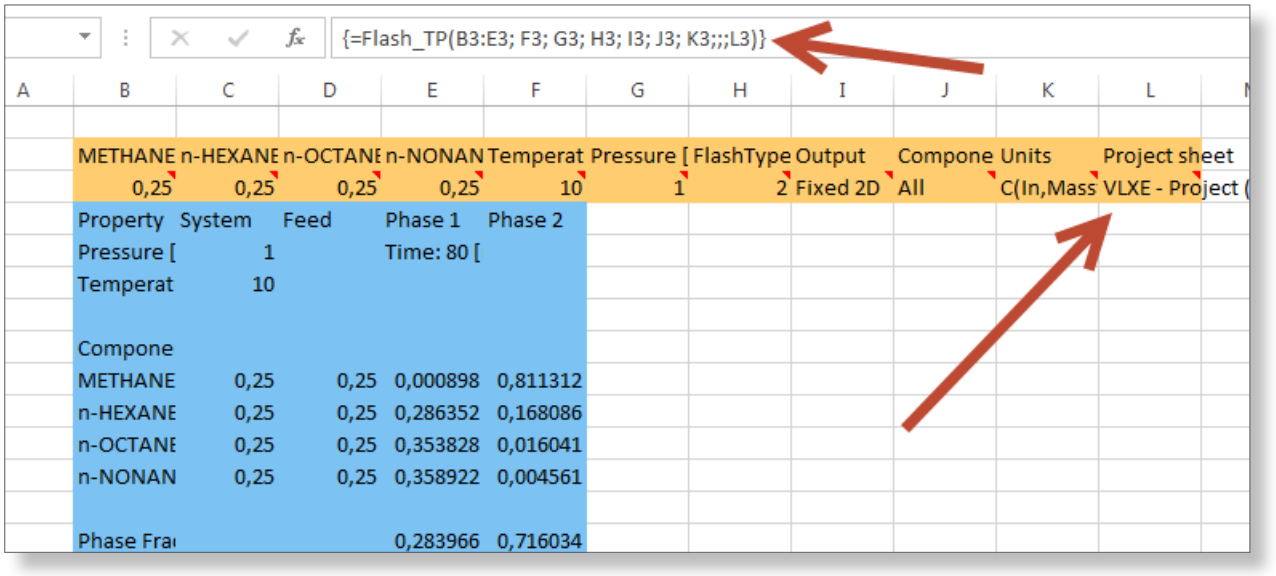


Note the selection on the bottom and the component list. Then click “OK” in the selection window.



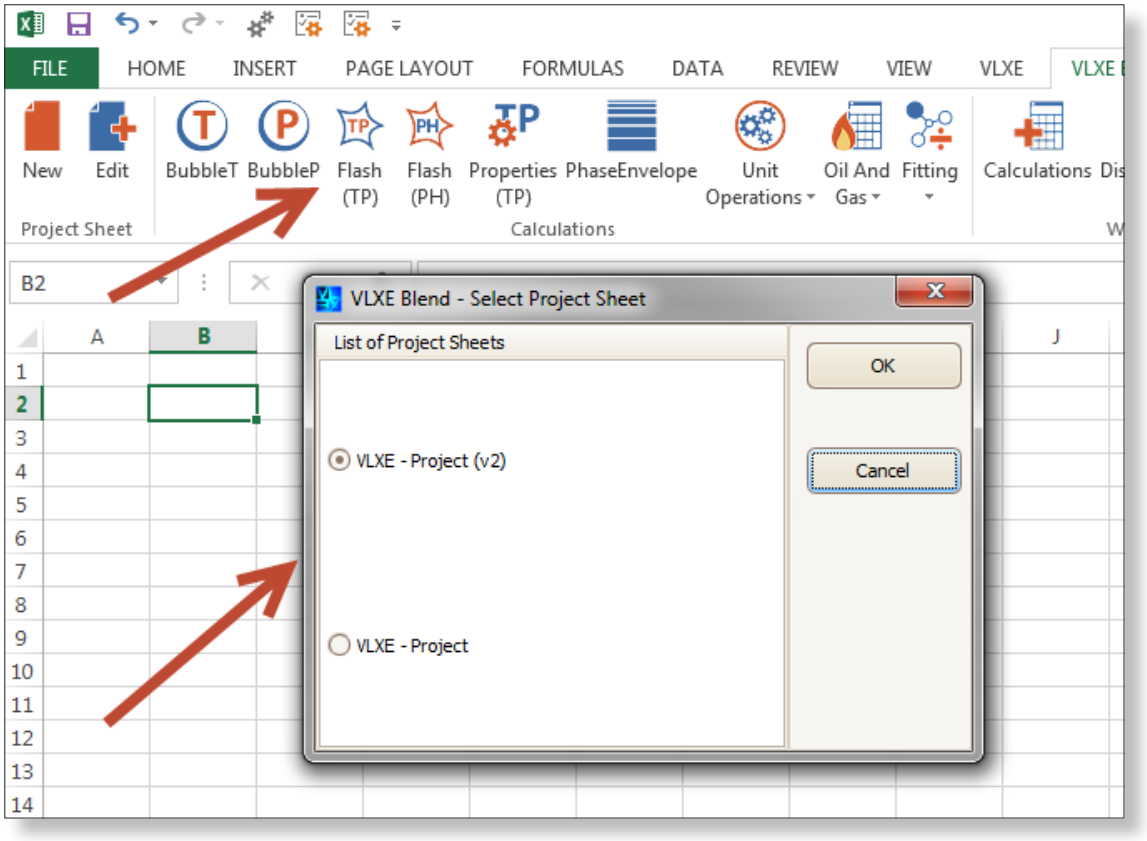
Note how the selected project sheet name has changed and the component list has changed with it.

Now complete the wizard to generate the flash result. Once done, note how the "ProjectSheet" is now in use.



3.7.2 Using the Shortcut on the VLXE Blend ribbon: "Phase envelope"

If you are creating a new flash calculation using the shortcut provided on the VLXE Blend ribbon, press the "Shift" key before clicking on the "Flash" icon. This will allow you to select the project sheet. If you do not press "Shift", the default project sheet is used. In other words, the wizard will not include the "ProjectSheet" in the calculation setup.

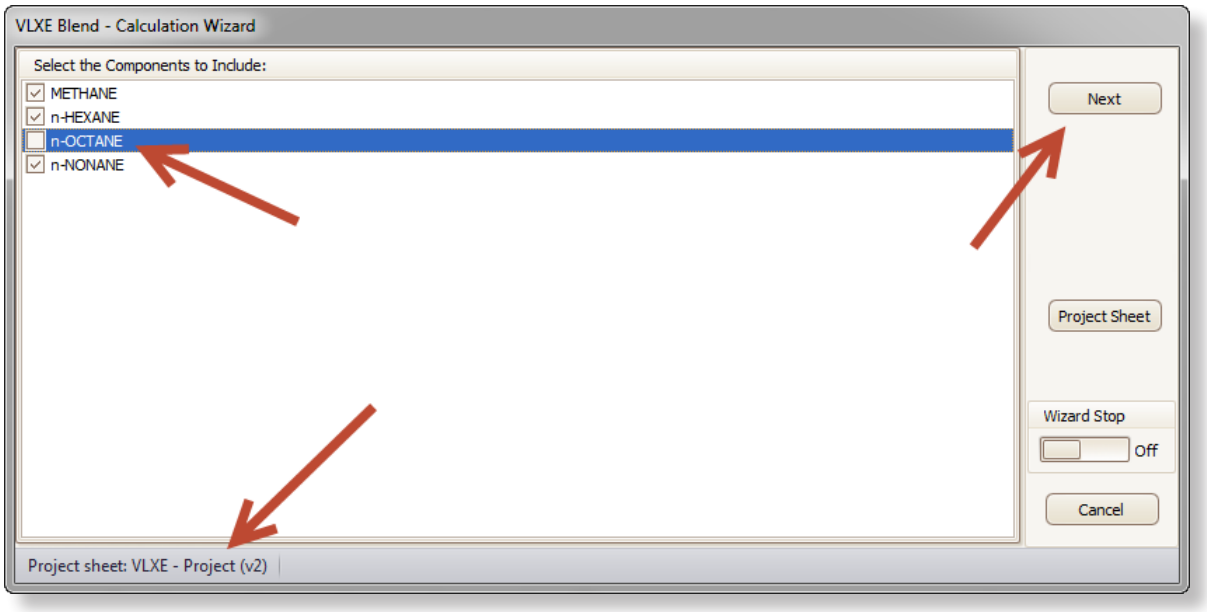


3.8 Select Components Included in a Calculation

A calculation can pick the components to be included from the project sheet. This is done using the "Components" argument. The argument is always included and is set by default to "All". It can be changed by hand or using the built-in wizard once the calculation is created or on the first page of the calculation wizard. To illustrate, we will use the 4 component project sheet just created.

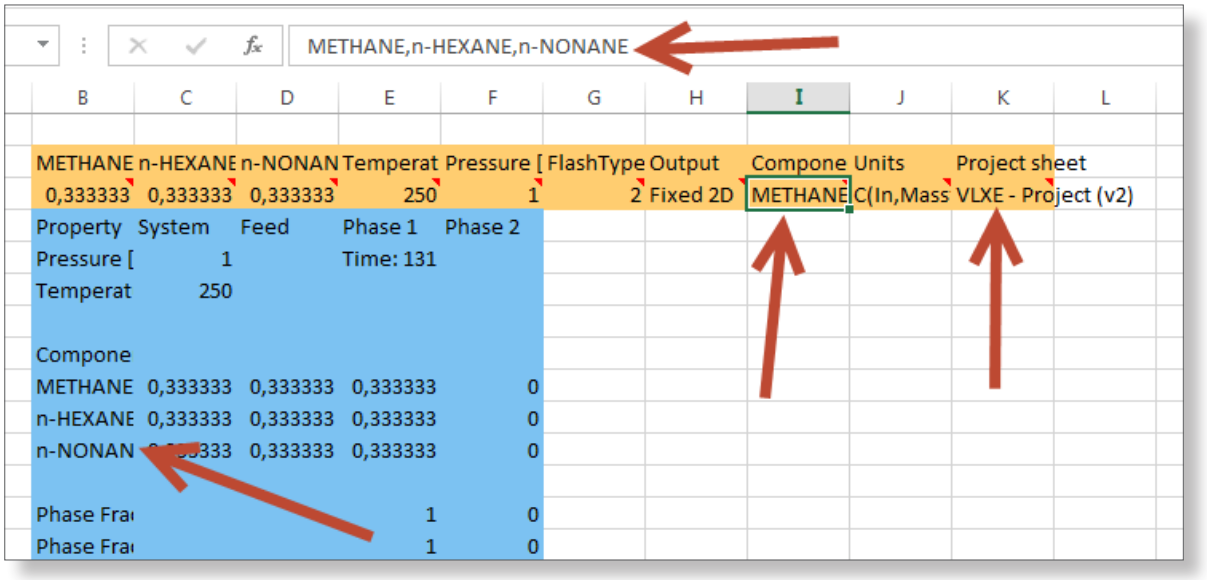
3.8.1 Change in calculation wizard

Go to a blank sheet and open the calculation wizard. In the window remove the checkmark from "n-Octane".



Finish the wizard to set up a flash calculation. In the output note the project that has been used, the components argument and the components included in the flash calculation.

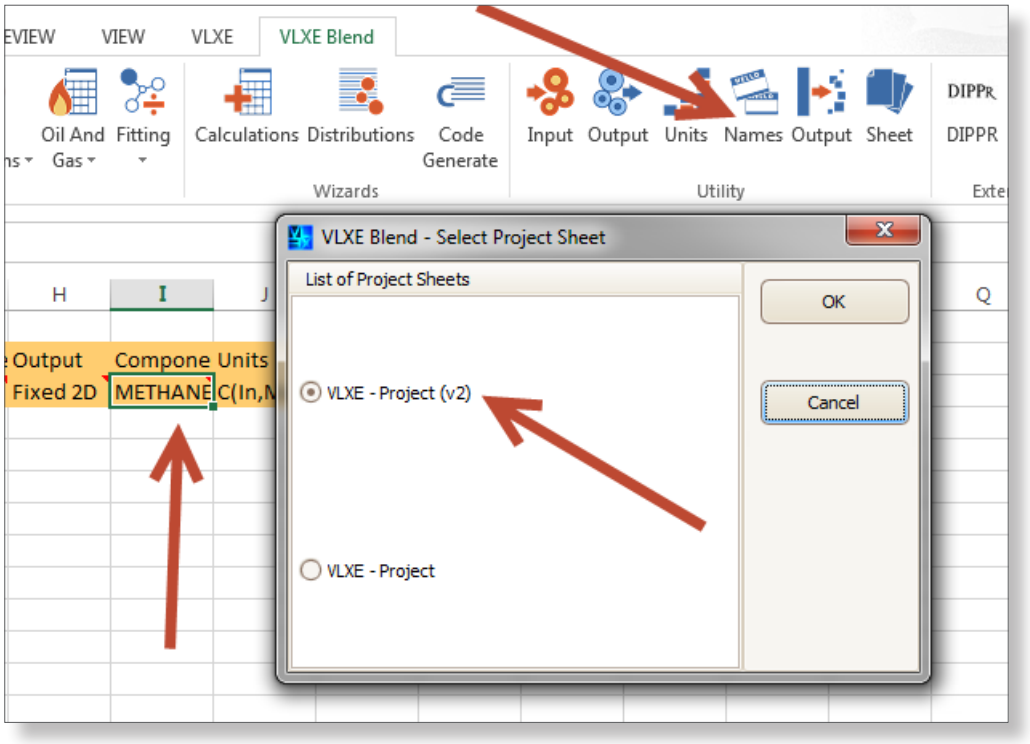
Of the 4 components in the project, only the 3 selected are now used.



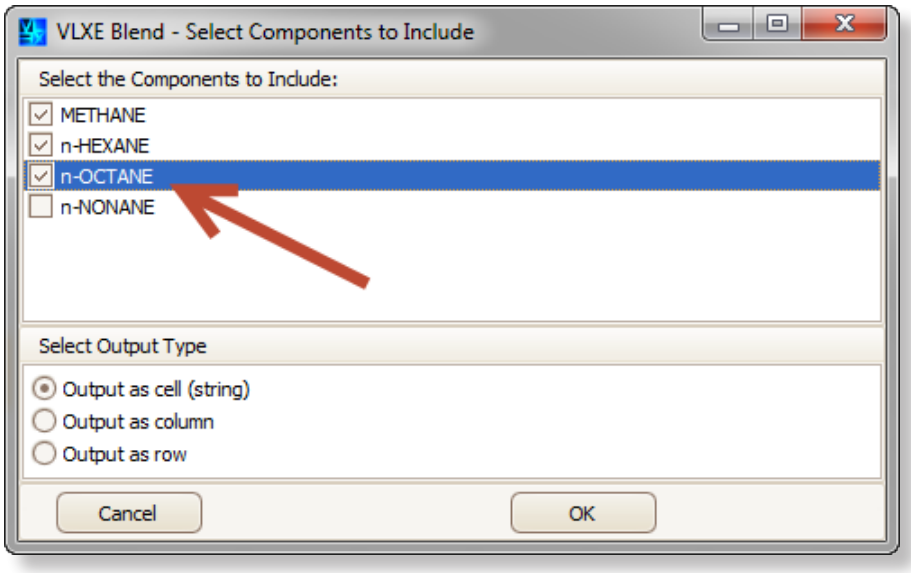
3.8.2 Change after calculation is created

Once a calculation is created, the component list can be altered simply by changing the string used as the component argument. It can be changed either by hand or using the "Names" wizard.

To illustrate, click on the component cell in the calculation just created. Then hold down the shift key and click on "Names" on the VLXE Blend ribbon.

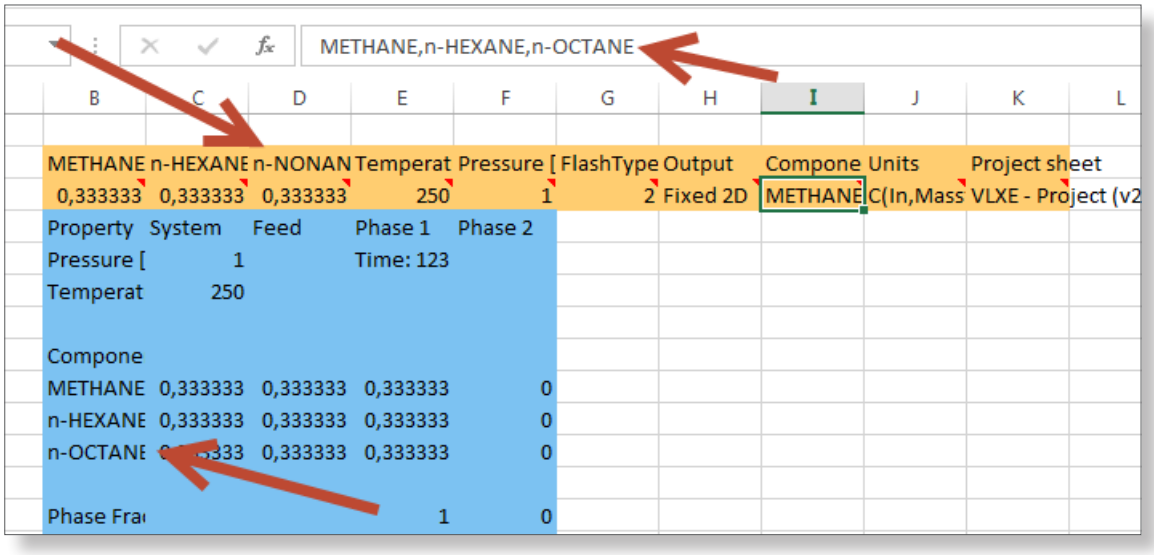


In the new window, select the first 3 components, thereby changing the components to be used in the flash calculation.



Select "OK" and note how the calculation is updated using the new component list.

Warning: Also note how the labels above the feed do not change. It is very important to remember to change these by hand.

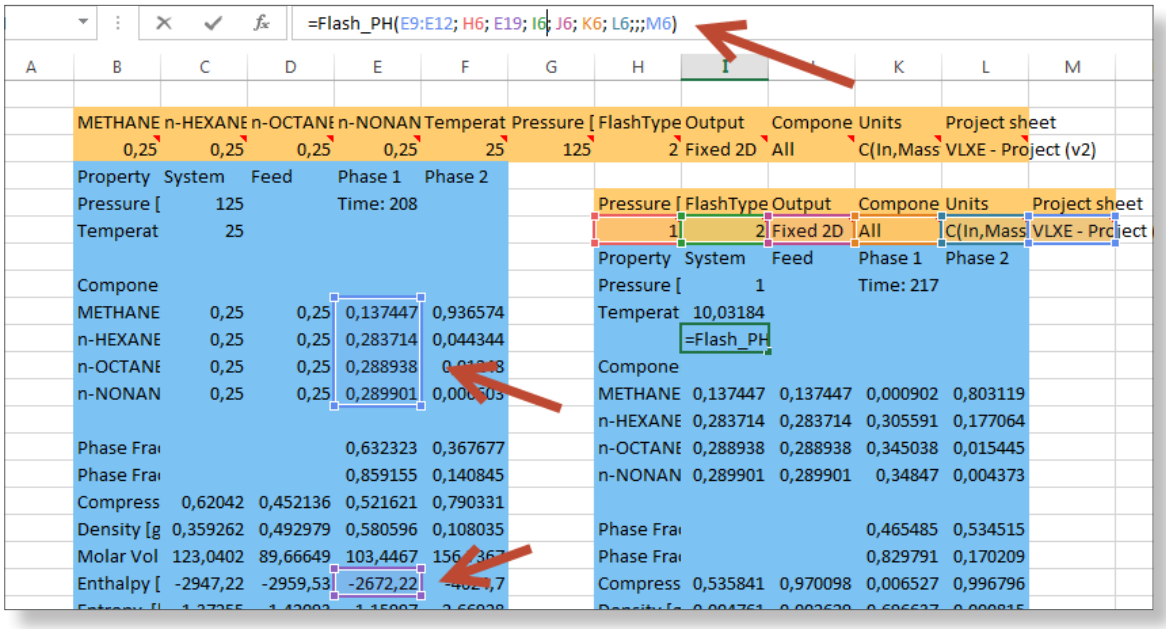


3.9 Link Flash Calculations

A common use of VLXE Blend is to link 2 or more calculations, thereby creating a small simulation. VLXE Blend cannot replace a full simulator, but it makes it very easy to investigate the relevant part of the process.

To illustrate we will create a simple example using the 4 component system from before. We will link 2 flash calculations to simulate a separation. The heavy phase from the first flash is sent to the second flash. Once linked, we will use Excel's Goal-seek to solve for an inlet pressure.

In a blank sheet, create a new T/P flash using the calculation wizard. Then next to it, create a P/H flash. Now change the feed and enthalpy link for the second flash so that it uses the output from the first flash.

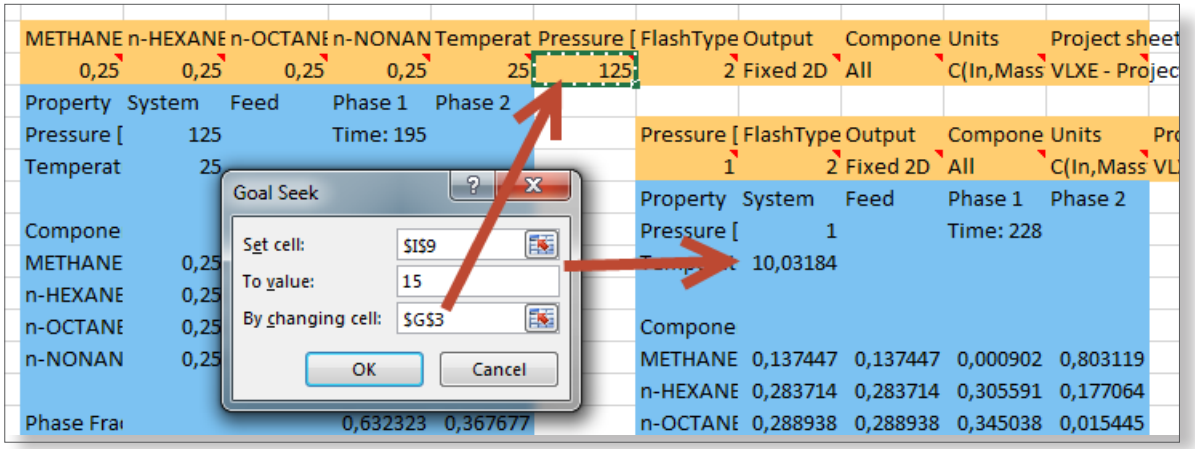


We have now created a simple separation and can work with the input to see the effect.

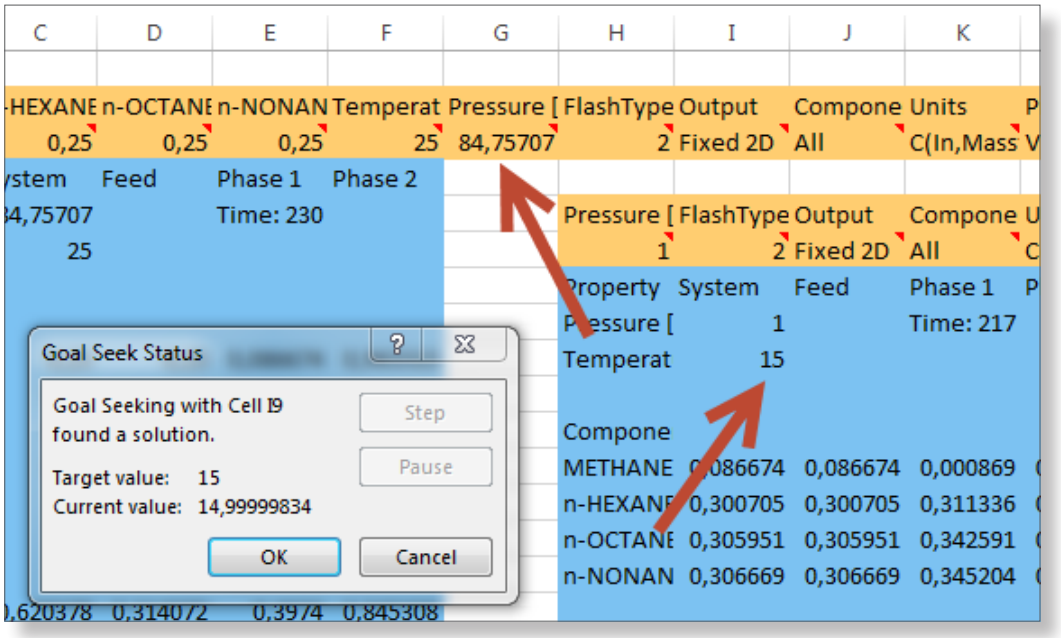
3.10 Using Excel´s Goal Seek feature to solve simulation

Once we have the calculations linked, we can use Excel's built-in Goal Seek feature to solve, for example, for outlet temperature. We can thereby converge a simulation. As an example, we will use Goal Seek to find the pressure in the first flash such that it yields a temperature of 25°C in the second flash.

Open Goal Seek under Data/"What-If Analysis".



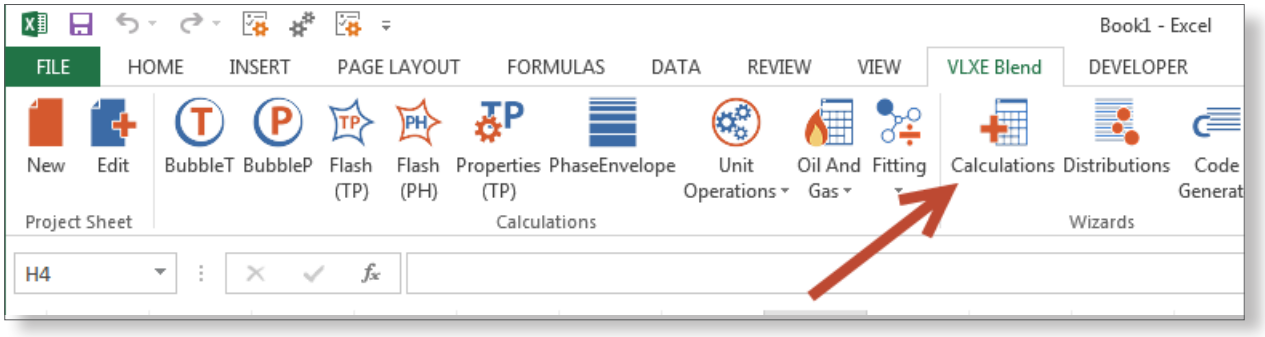
Select "OK" and the solver will run for a few seconds. The cells are automatically ajusted.



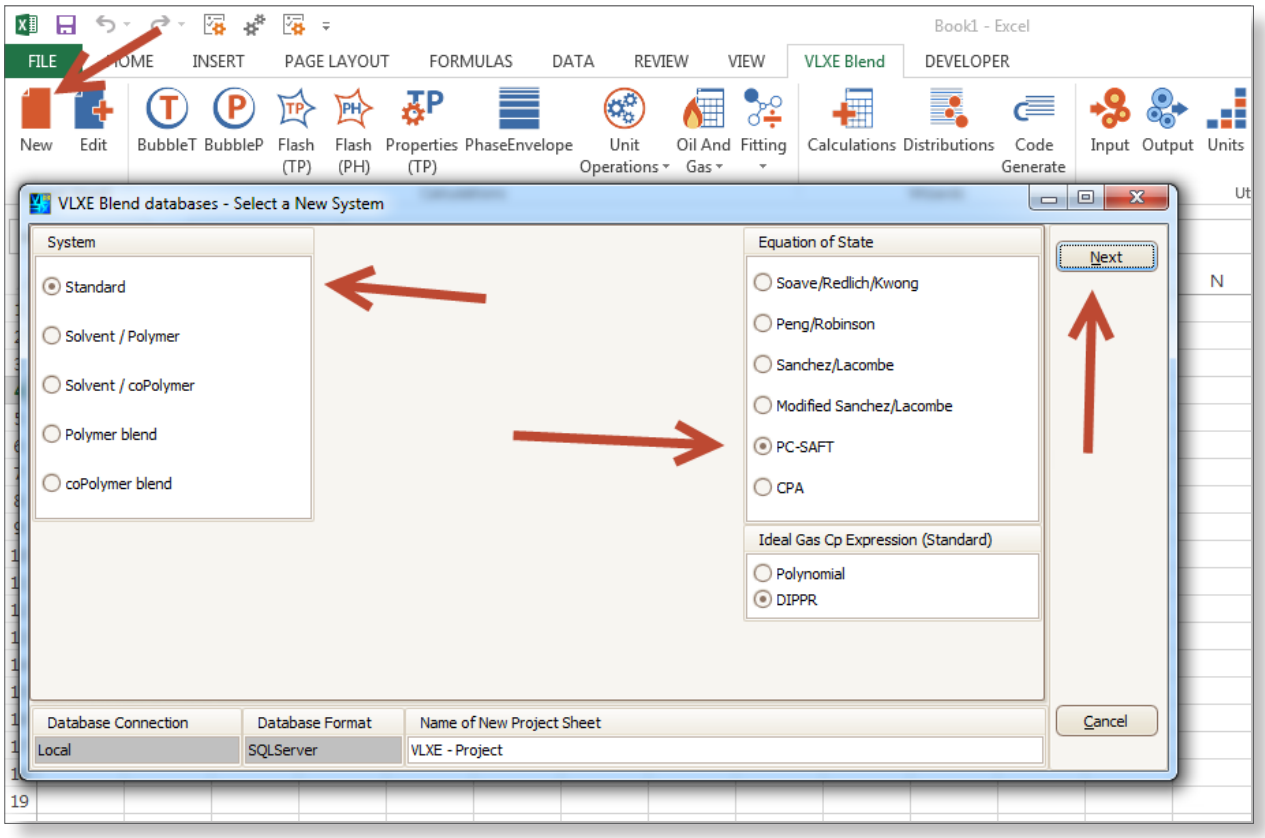
4) Association Components

This chapter describes how to calculate the properties of components that form an association with each other in the liquid and vapor phases. This is described by the use of a methanol cyclohexane example. A step-by-step procedure is shown below.

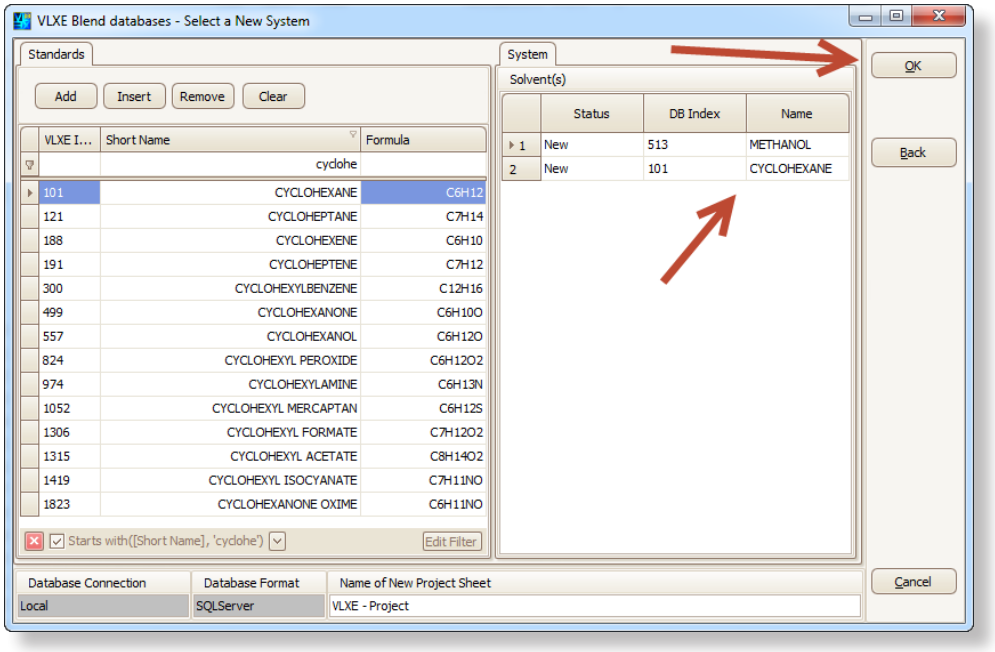
1. Open an Excel sheet.
Click on "New" from the database.



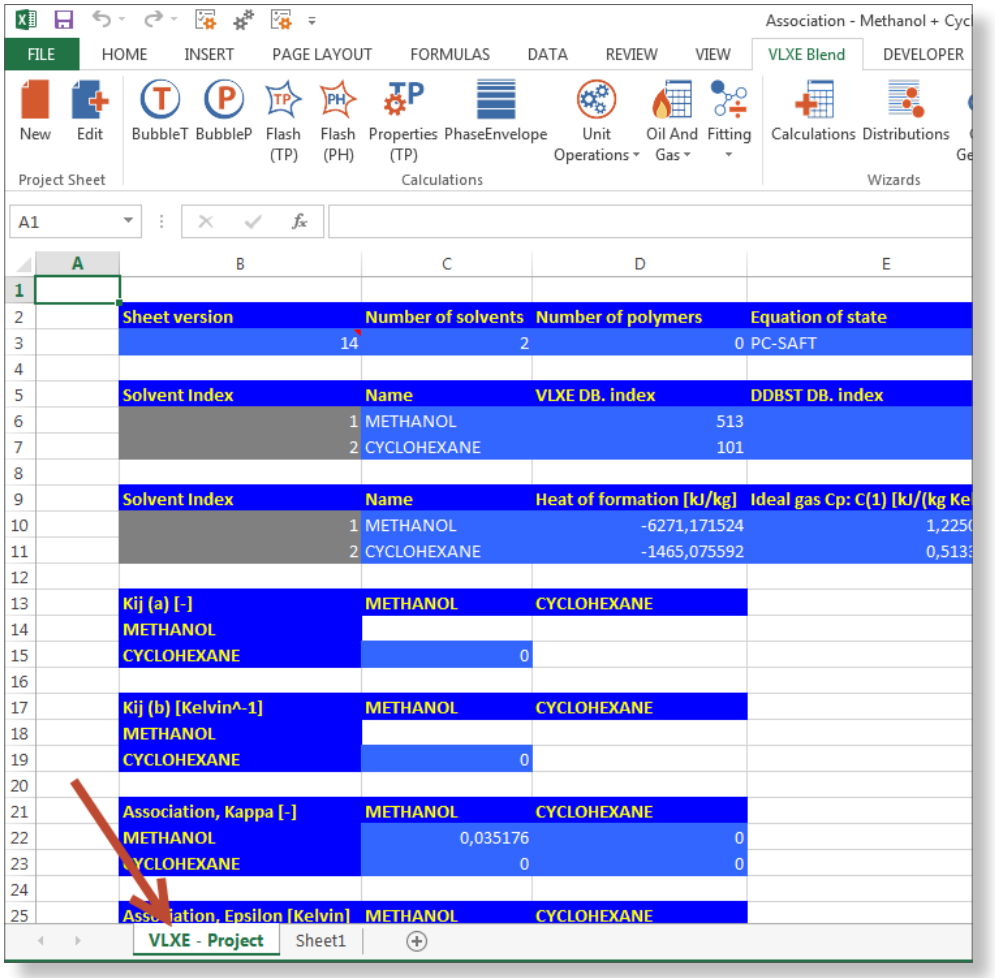
2. Select the type of system, Equation of State and ideal gas Cp expression (solvents).
For a methanol cyclohexane mixture, PC-SAFT equation of state and standard system is selected with polynomial ideal gas Cp expression.



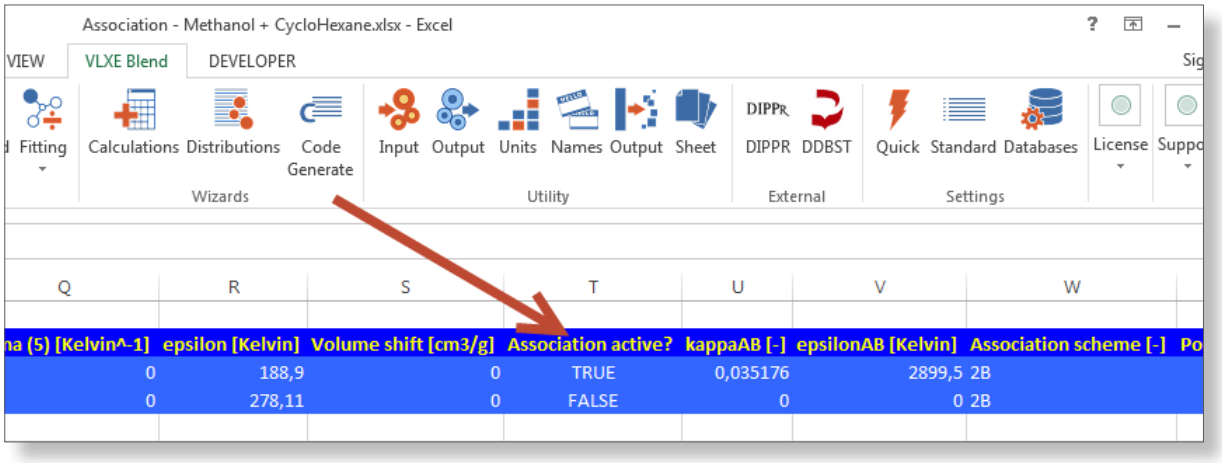
3. Click “Next” and add solvents from the databank to define the system.
Select methanol and cyclohexane from the databank. Selected components are shown in the figure below.



4. Click “Next” and all the results will be displayed in an Excel sheet.



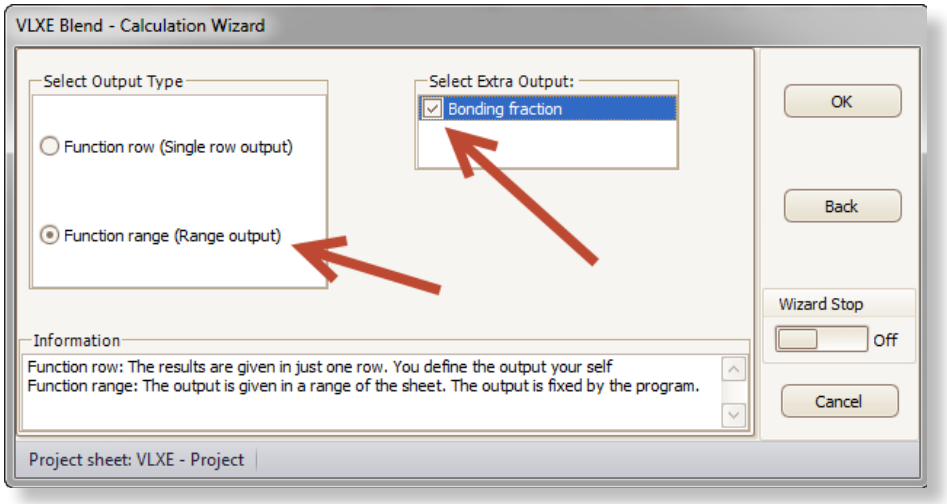
5. PC-SAFT equation of state with polynomial ideal gas Cp expression will also tell whether the solvent is associated or not. Also it tells something about the association scheme.



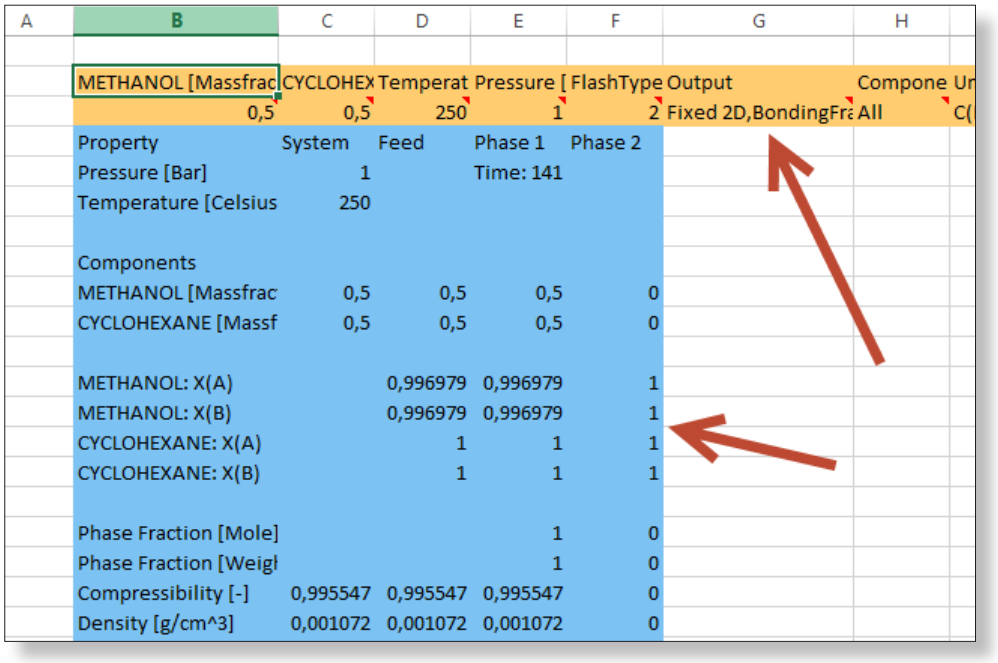
4.1 Bonding fraction as output

The bonding fraction can be part of the calculation output. A common reason for doing this is to compare with experimental data or simply to check how the bonding fraction moves with the input.

It is best seen as part of the standard 2D output. To illustrate, create a flash calculation using the calculation wizard. On the last page select as shown below:



Note that the bonding fraction is now included in the output. See how it includes A and B since “2B” scheme is used plus how cyclohexane has a bonding fraction of 1 since it does not associate.

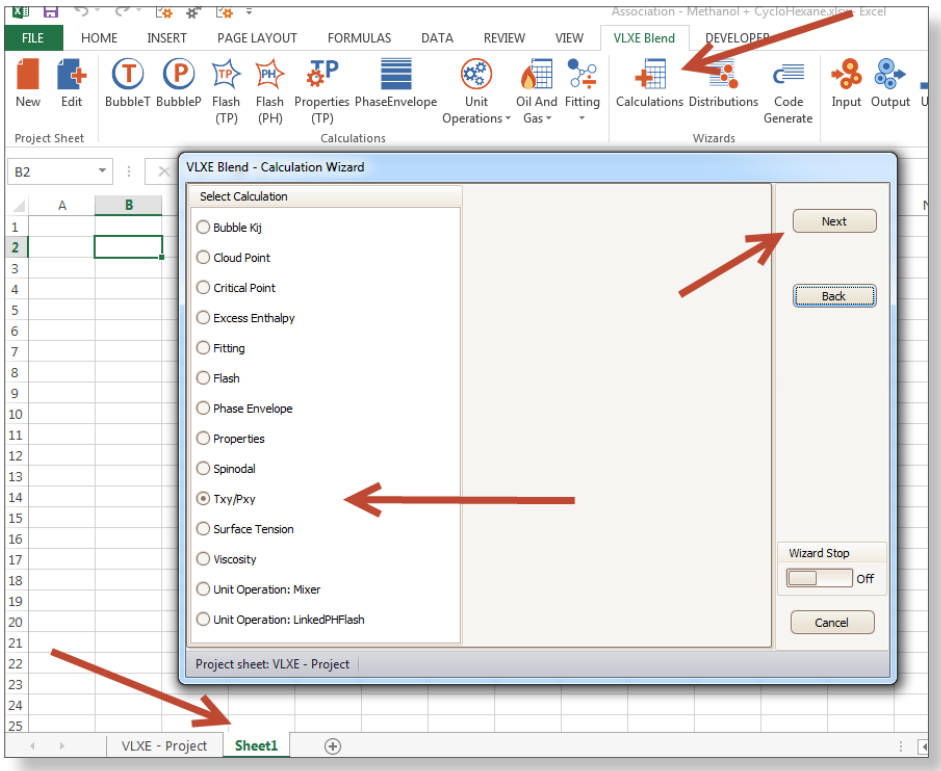


	METHANOL [Massfrac	CYCLOHEX	Temperat	Pressure [	FlashType	Output	Compone	Ur
	0,5	0,5	250	1	2	Fixed 2D,BondingFra	All	C(
	Property	System	Feed	Phase 1	Phase 2			
	Pressure [Bar]	1		Time: 141				
	Temperature [Celsius	250						
	Components							
	METHANOL [Massfrac	0,5	0,5	0,5	0			
	CYCLOHEXANE [Massf	0,5	0,5	0,5	0			
	METHANOL: X(A)		0,996979	0,996979	1			
	METHANOL: X(B)		0,996979	0,996979	1			
	CYCLOHEXANE: X(A)		1	1	1			
	CYCLOHEXANE: X(B)		1	1	1			
	Phase Fraction [Mole]			1	0			
	Phase Fraction [Weigl			1	0			
	Compressibility [-]	0,995547	0,995547	0,995547	0			
	Density [g/cm^3]	0,001072	0,001072	0,001072	0			

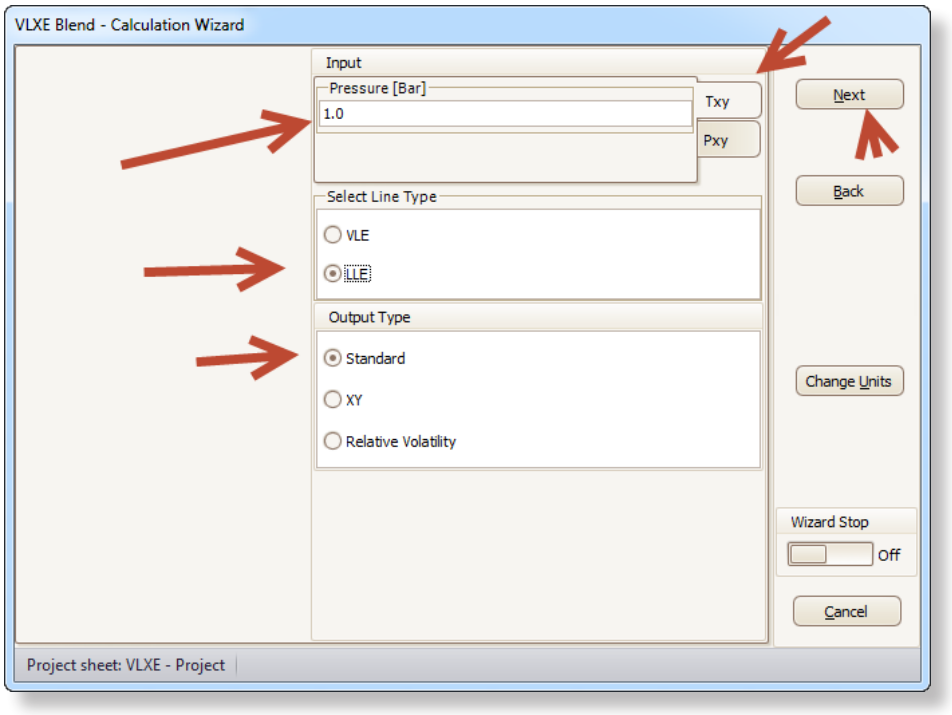
4.2 Txy/Pxy Calculations

1. When the system is defined and all the parameters are loaded into an Excel spreadsheet, the next step is to make some calculations.
Click on the standard wizard and go to “Calculations”.

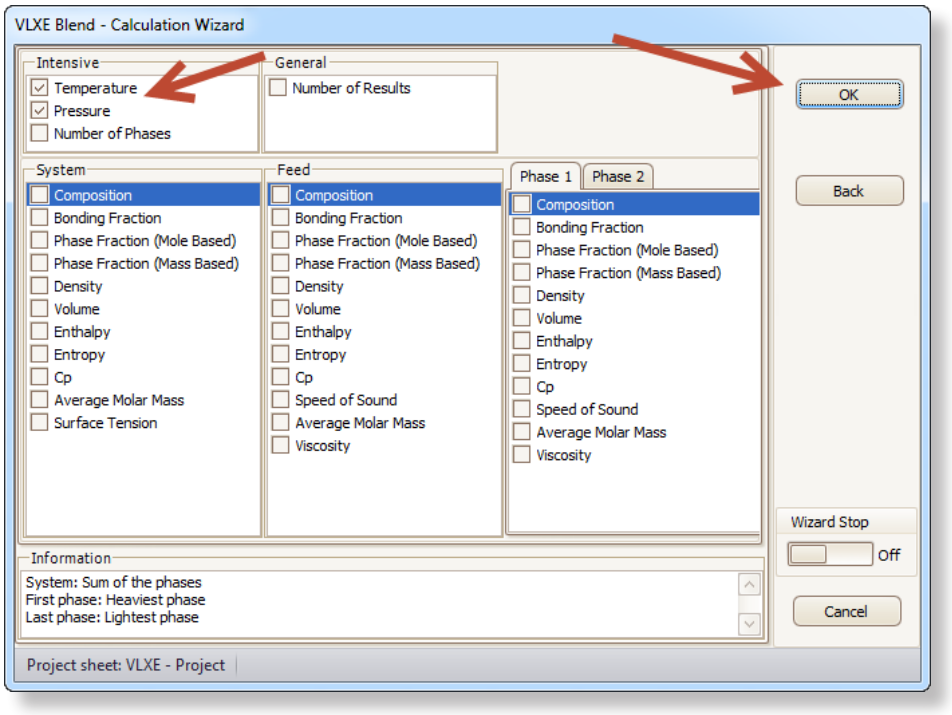
2. Select “Txy/Pxy” from the calculation wizard and click “Next”.



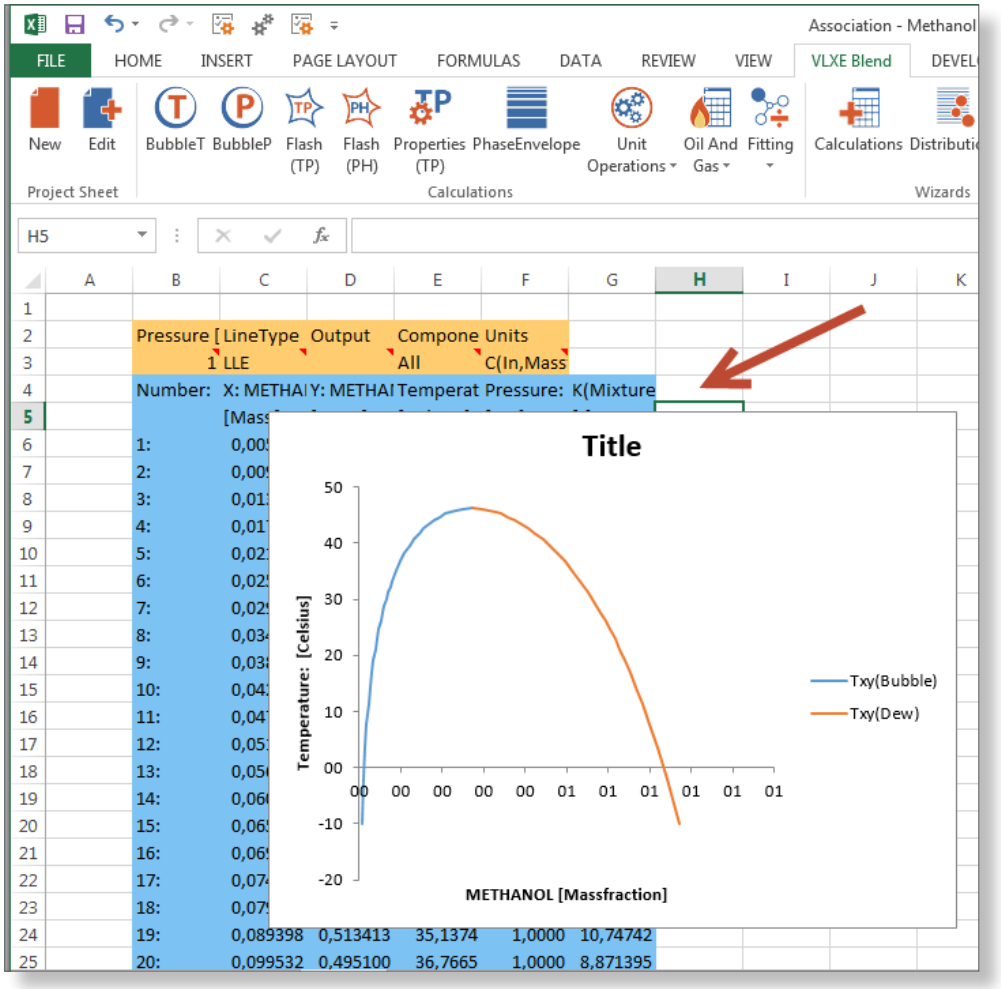
3. Give the pressure for the Txy calculation or the temperature for a Pxy calculation.
For this example a pressure of 1 Bar is given for the Txy calculation. Select an LLE type of curve, standard output and then click “Next”.



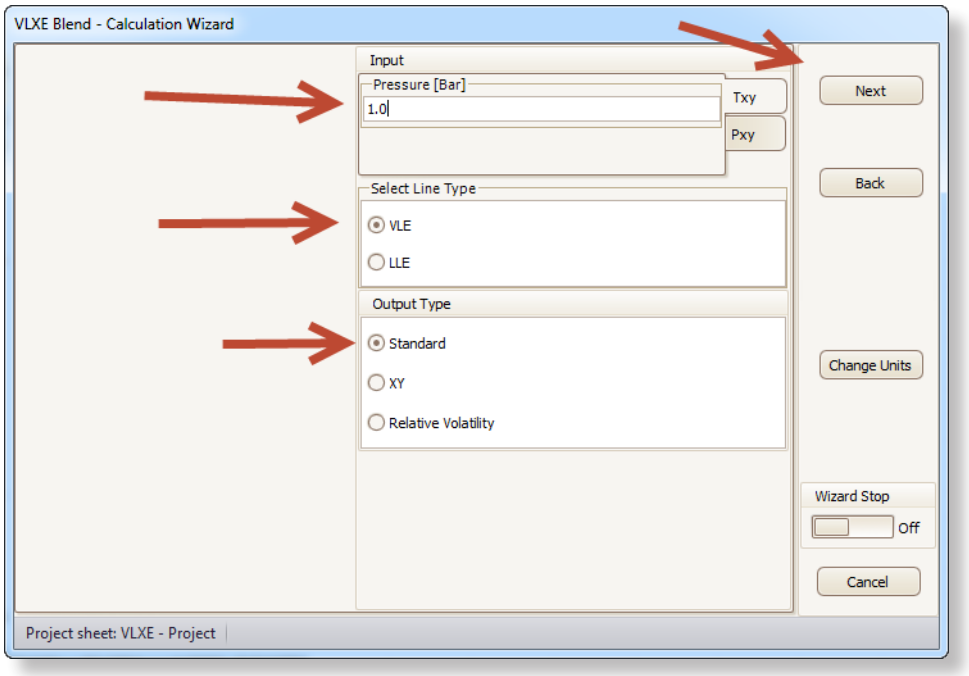
4. Select “Temperature” and “Pressure” and click “OK”.



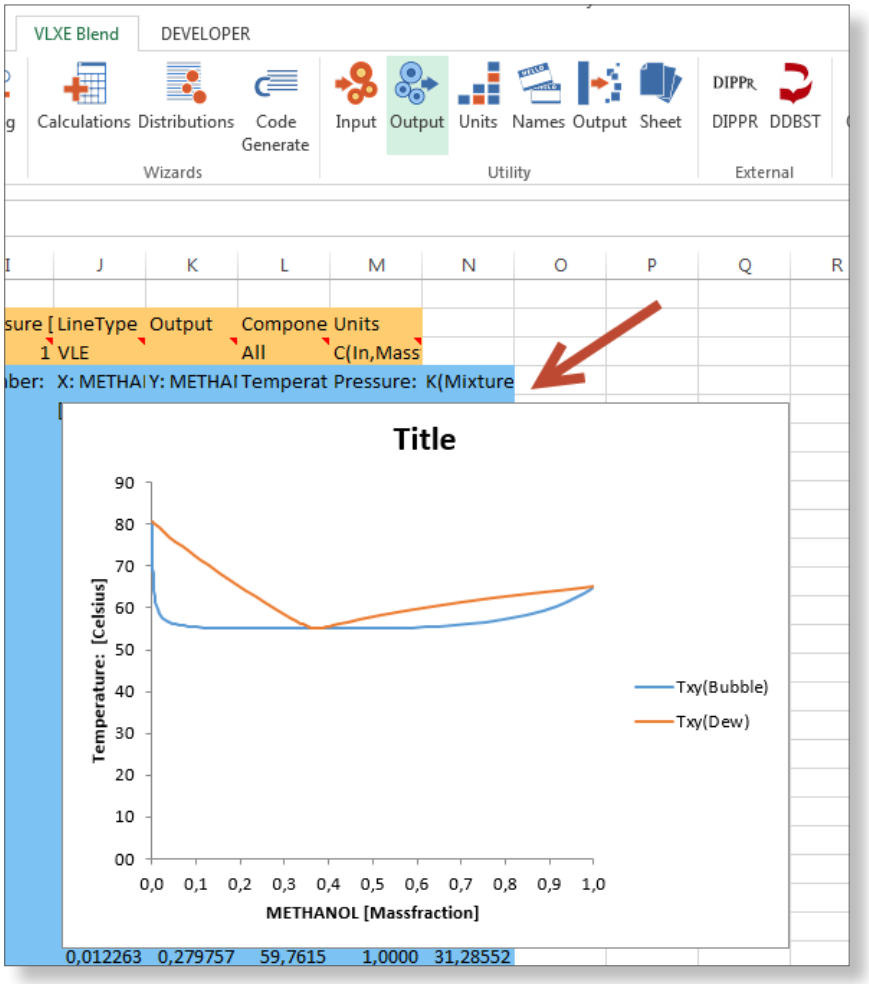
5. Bubble and dew point temperature, with respect to methanol composition, is plotted in a graph.



6. In a similar way, the VLE curve can be drawn by selecting VLE line type instead of LLE. All the other steps will remain the same as shown above.



7. The corresponding results in graphical form for VLE are shown below.



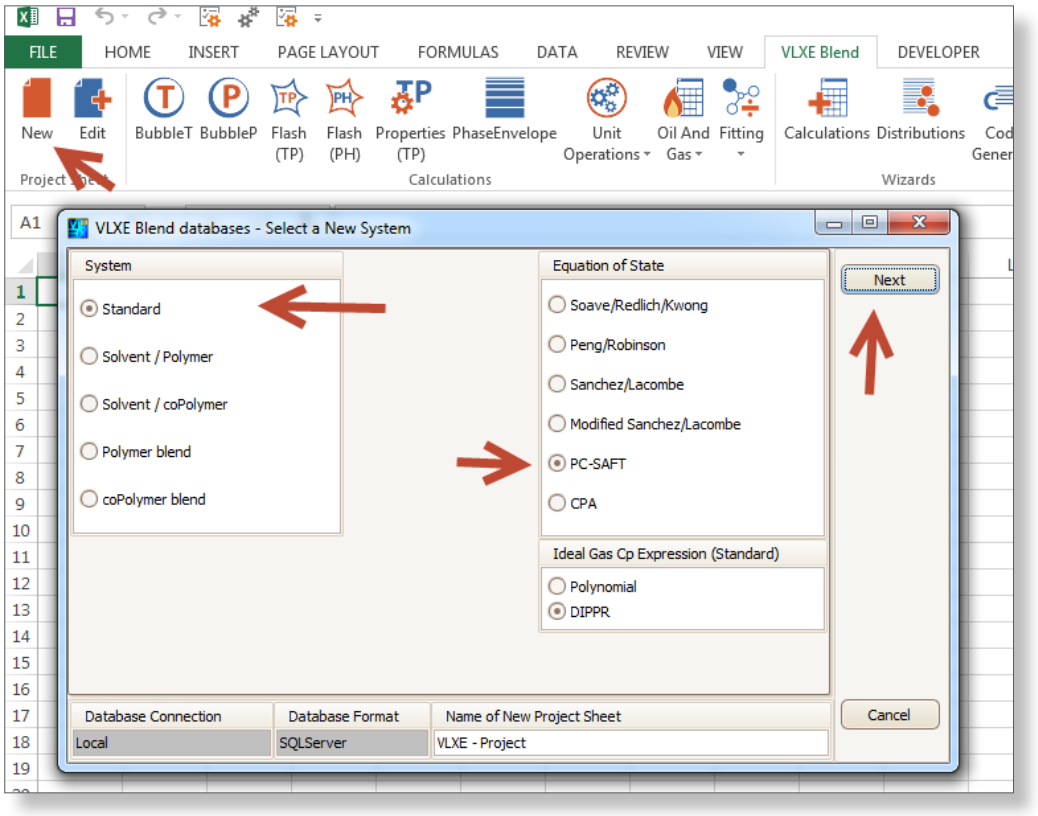
8. Effect of bubble point and dew point with respect to methanol composition with both LLE and VLE can also be plotted in the same graph. Just copy one graph, and paste it into the other graph with minor changes in axis in order to have a better view.

5) Polar Components

This chapter describes how to calculate the properties of components that form an association with each other in the liquid and vapor phases. This is best described by a methanol cyclohexane example. A step-by-step procedure is shown below.

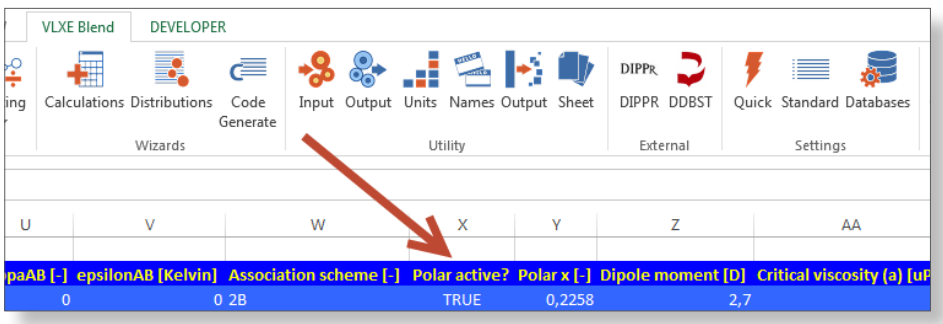
Polar molecules have slightly positive and slightly negative charged ends. This section deals with the system that contains polar molecules. An example of an acetone n-hexane mixture will be described here.

1. Set up or define the system. Select "Standard", choose "PC-SAFT" equation of state, select "Polynomial" ideal gas Cp expression and click "Next".



2. Define the components from the database and click "Next".

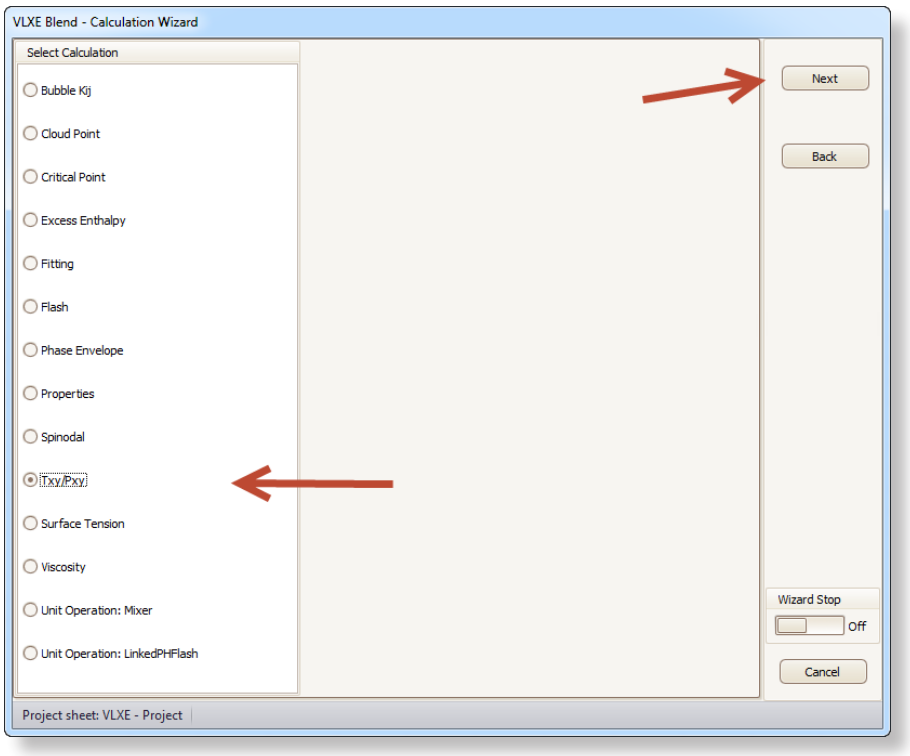
3. All the parameters are loaded into an Excel spreadsheet. For a system containing polar compounds an Excel spreadsheet is shown below that contains three additional terms i.e. Dipole moment, Polar coordinate and Polar active.



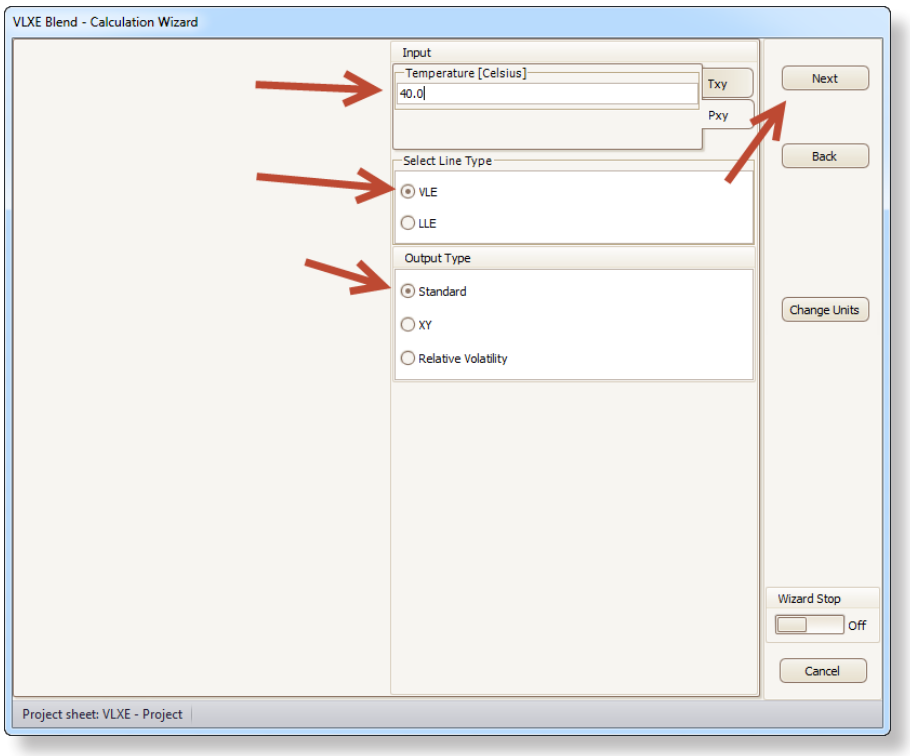
5.1 Pxy Calculations

As an example, the effect of pressure with composition is shown below. Other calculations can also be performed in the same manner as was shown for other solvent systems above.

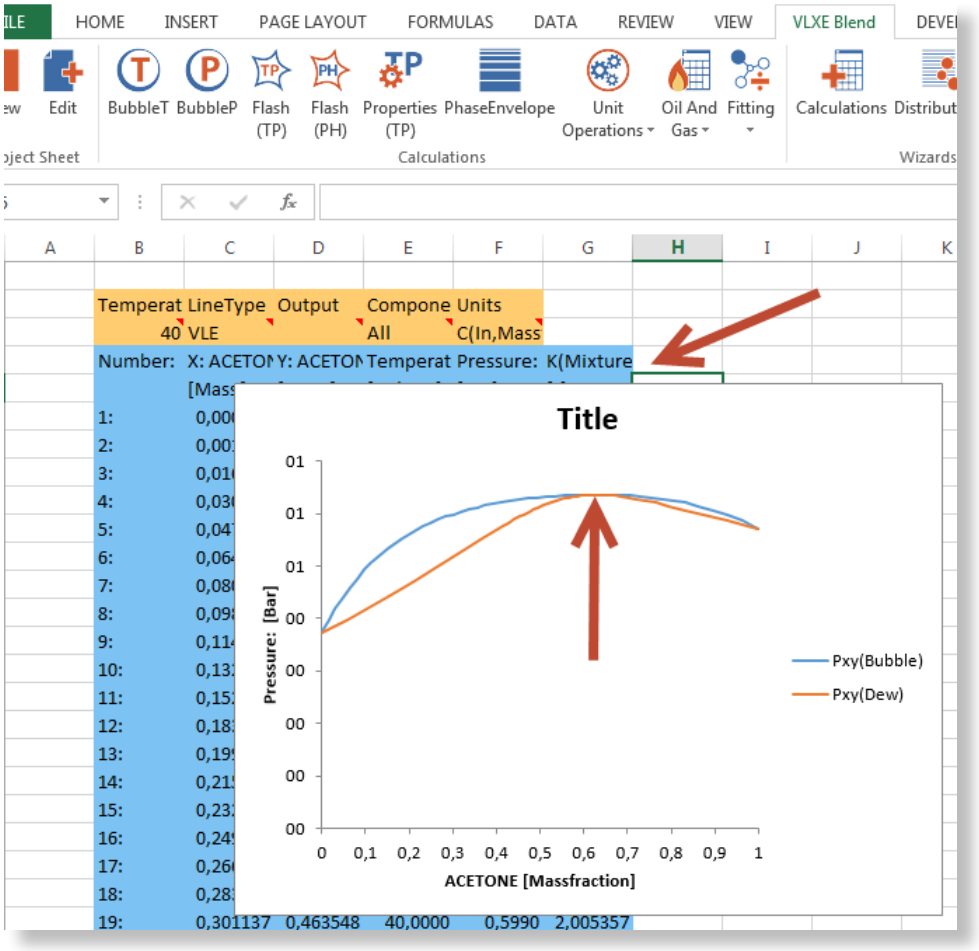
1. Start from the Calculation Wizard, click on “Calculations”, then select “Txy/Pxy” from the Calculation Wizard and click “Next”.



2. Click on “Pxy”, provide an input temperature, select VLE line type and standard output type and then click “Next”.



3. Click "Ok" and a graph between Acetone mass fraction against pressure is plotted. From the figure below it can clearly be seen that this mixture of acetone and n-hexane forms an azeotrope.



6) Polymer

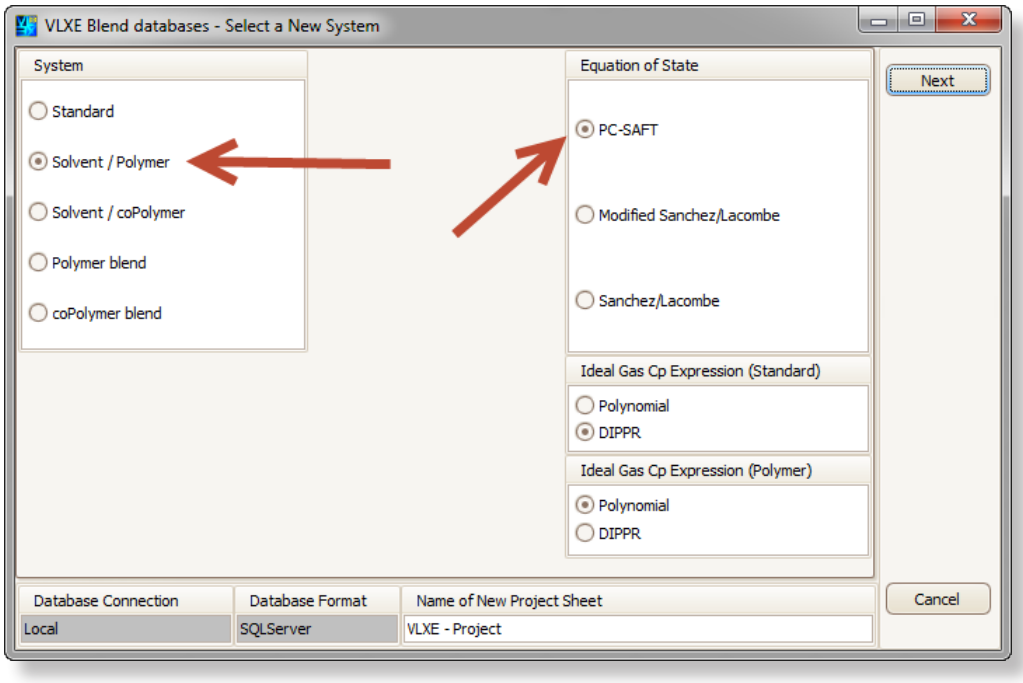
Polymers are the core part of VLXE Blend. As the only PVT package in the world that offers a full range of models and robust calculations.

The main advantages of VLXE Blend is that it makes polymer calculations just as simple as any other ones. Here there is no difference between a poly-disperse polymer system and a n-Hexane system. The only place where you will notice any difference is for poly-dispersity and copolymers. In these cases, a bit more in and out-put is needed.

By now you know how to use VLXE Blend, so the focus now is on the small differences in in- and out-put , and additionally an overview of the polymer calculations in VLXE Blend is provided.

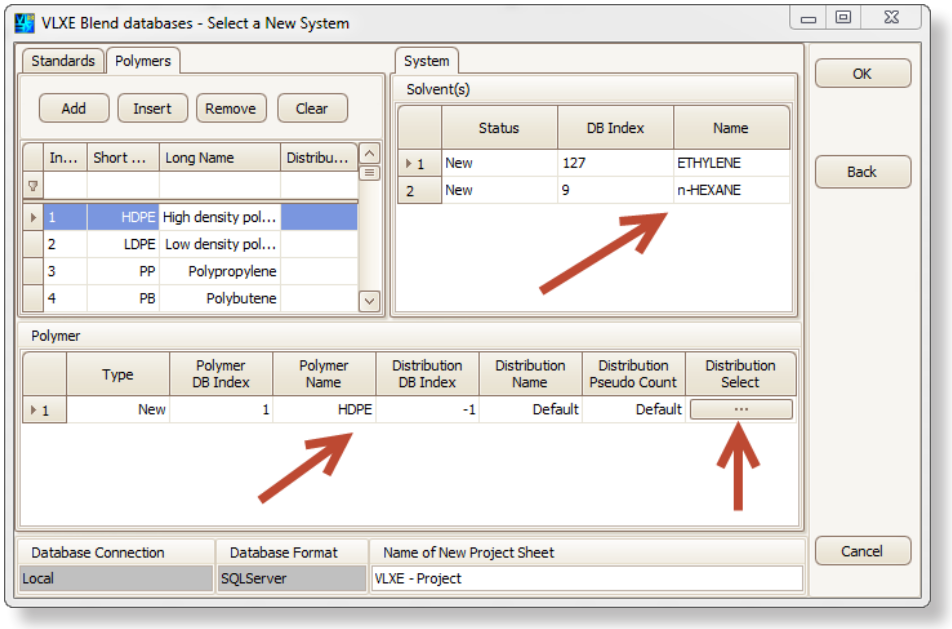
6.1 Create a new Polymer Project

Create a new Excel file and select “New” on the VLXE Blend ribbon. Select as shown below.

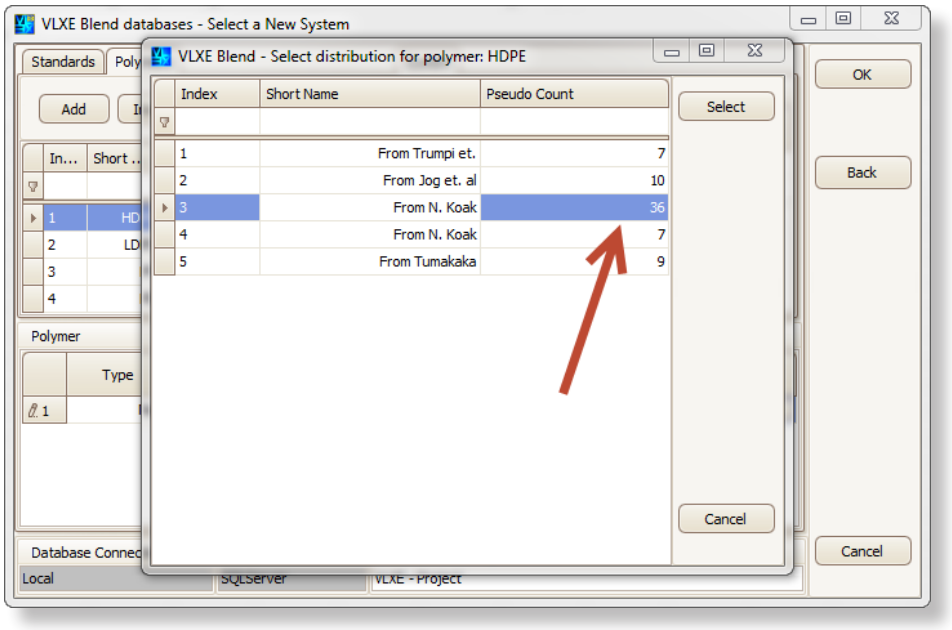


On the next page, select Ethylene and n-Hexane as solvents and HDPE as the polymer. So as to include a distribution for the polymer, select “Distribution select”.

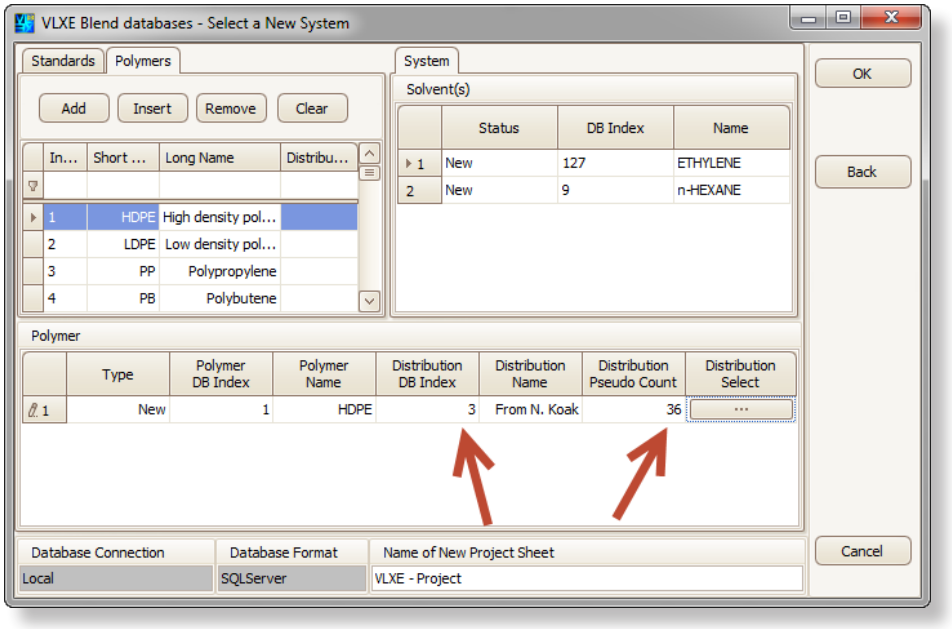
Note that if no distribution is selected here, a default value for a mono-disperse polymer is used. The molar mass can then be changed once the project sheet is created.



In the dialog that opens, select “From N. Koak”.

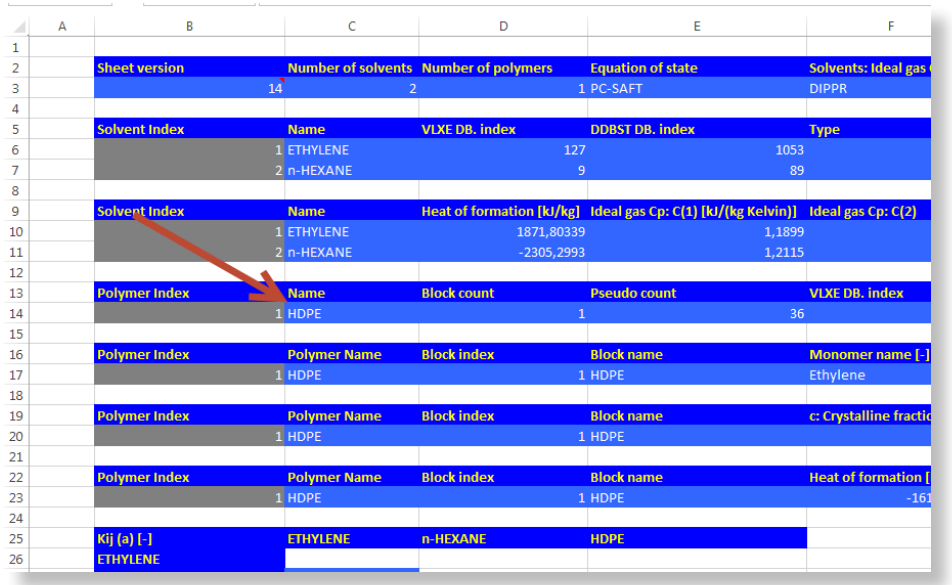


This distribution is now attached to the selected polymer.



Click on "OK" to create the project sheet.

All the parameters and properties of the system with the two solvents (Ethylene and n-Hexane) and the polymer (HDPE) are loaded into the Excel sheet. Take a look at the sheet to see how the polymer information is included:



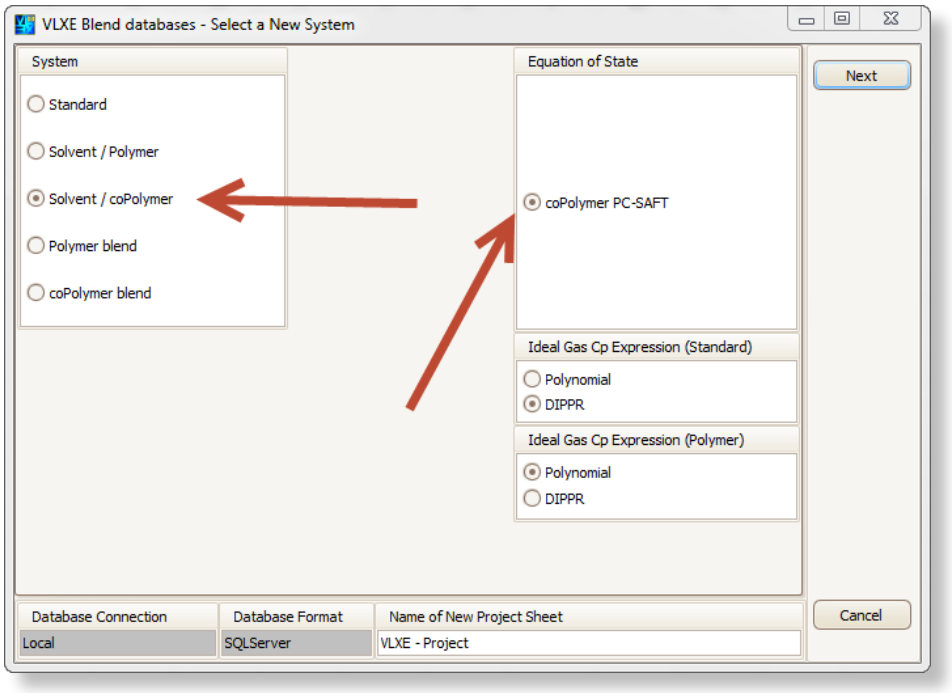
	A	B	C	D	E	F
1						
2		Sheet version	Number of solvents	Number of polymers	Equation of state	Solvents: Ideal gas
3		14	2	1	PC-SAFT	DIPPR
4						
5		Solvent Index	Name	VLXE DB. index	DDBST DB. index	Type
6		1	ETHYLENE	127	1053	
7		2	n-HEXANE	9	89	
8						
9		Solvent Index	Name	Heat of formation [kJ/kg]	Ideal gas Cp: C(1) [kJ/(kg Kelvin)]	Ideal gas Cp: C(2)
10		1	ETHYLENE	1871,80339	1,1899	
11		2	n-HEXANE	-2305,2993	1,2115	
12						
13		Polymer Index	Name	Block count	Pseudo count	VLXE DB. index
14		1	HDPE	1	36	
15						
16		Polymer Index	Polymer Name	Block index	Block name	Monomer name [-]
17		1	HDPE	1	HDPE	Ethylene
18						
19		Polymer Index	Polymer Name	Block index	Block name	c: Crystalline fracti
20		1	HDPE	1	HDPE	
21						
22		Polymer Index	Polymer Name	Block index	Block name	Heat of formation [
23		1	HDPE	1	HDPE	-161
24						
25		Kij (a) [-]	ETHYLENE	n-HEXANE	HDPE	
26		ETHYLENE				

The distribution information for the polymer is given at the end.
Note the range of molar mass. From 3300 g/mole to 1.7E6 g/mole.
VLXE Blend has no limit on molar mass.

6.2 Create a new Copolymer Project

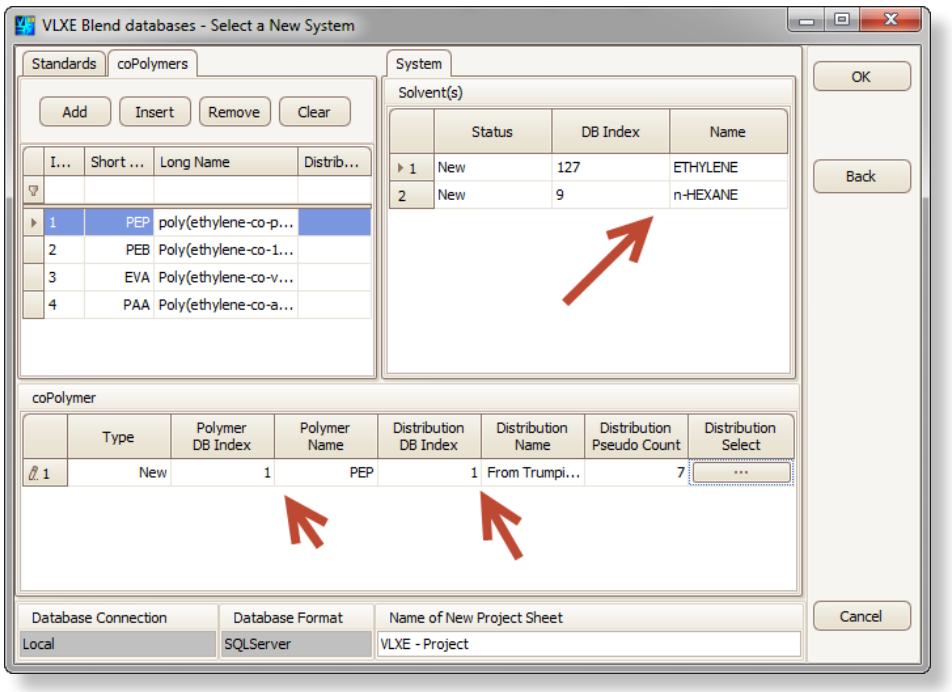
The procedure for creating a new copolymer project sheet is the same as for a polymer system.

Select “New” on the VLXE Blend ribbon. In the database wizard select as shown below.



Click “Next”.

As an example, ethylene, n-hexane and PEP (polyethylenecopropylene) with a 7 pseudo-component distribution is used. Select those components as given below



Click “OK” to generate the project sheet.

Take a look at the project sheet and compare it to the one from before with a polymer. Note how extra rows are added due to the 2 blocks in the copolymer.

Solvent Index	Name	Heat of formation [kJ/kg]	Ideal gas Cp: C(1) [kJ/(kg Kelvin)]	Ideal gas Cp: C(2)	Ideal gas Cp
1	ETHYLENE	1871,80339	1,1899	3,3789	
2	n-HEXANE	-2305,2993	1,2115	4,0882	

Polymer Index	Name	Block count	Pseudo count	VLXE DB. index	DDBST DB. i
1	PEP	2	7	1	

Polymer Index	Polymer Name	Block index	Block name	Block Mass Fraction [-]	Monomer n
1	PEP	1	HDPE	0,5	Ethylene
1	PEP	2	PP	0,5	Propylene

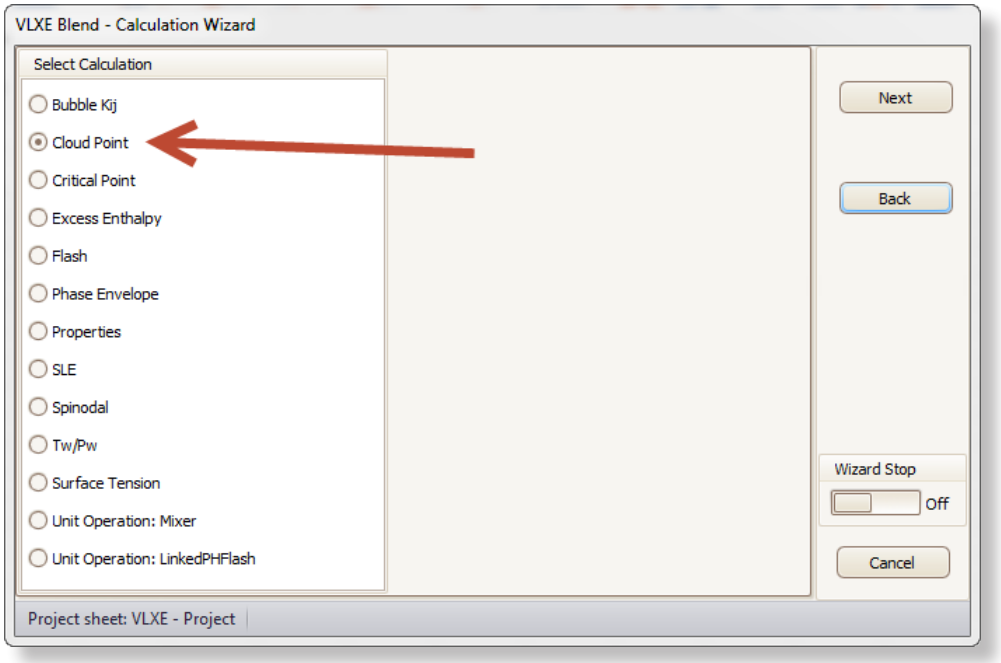
Polymer Index	Polymer Name	Block index	Block name	c: Crystalline fraction [-]	Enthalpy of
1	PEP	1	HDPE	0	
1	PEP	2	PP	0	

Polymer Index	Polymer Name	Block index	Block name	Heat of formation [kJ/kg]	Ideal gas Cp
1	PEP	1	HDPE	-1613,2549	
1	PEP	2	PP	0	

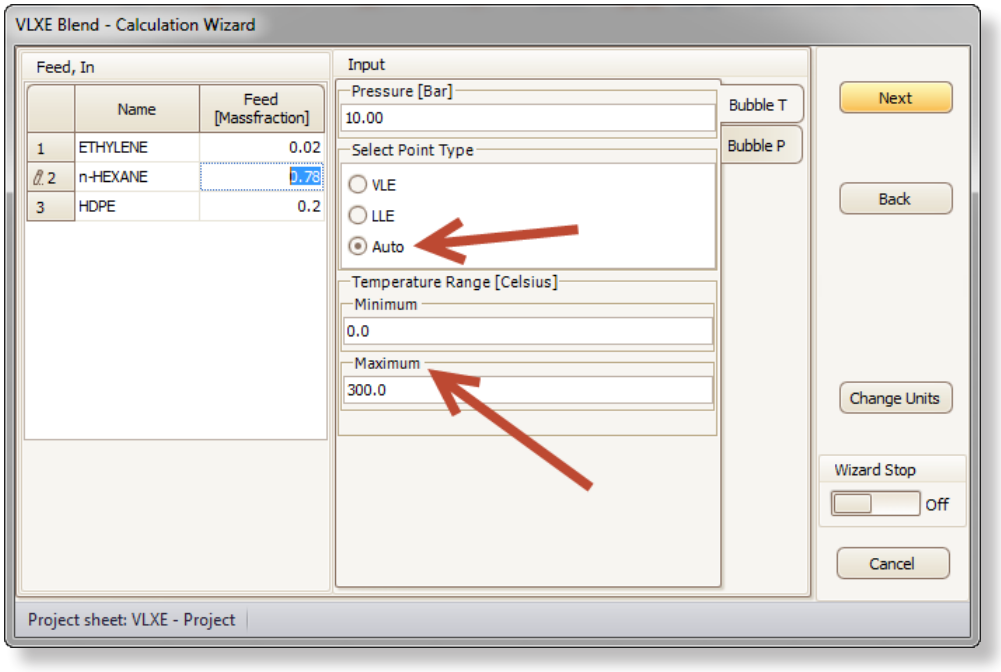
6.3 Cloud Point Calculation

We will now set up a cloud point calculation. VLXE Blend supports robust VLE and LLE cloud point calculations for any polymer system. When we go through the steps in the Calculation Wizard note how they are the same as for Methane + n-Hexane.

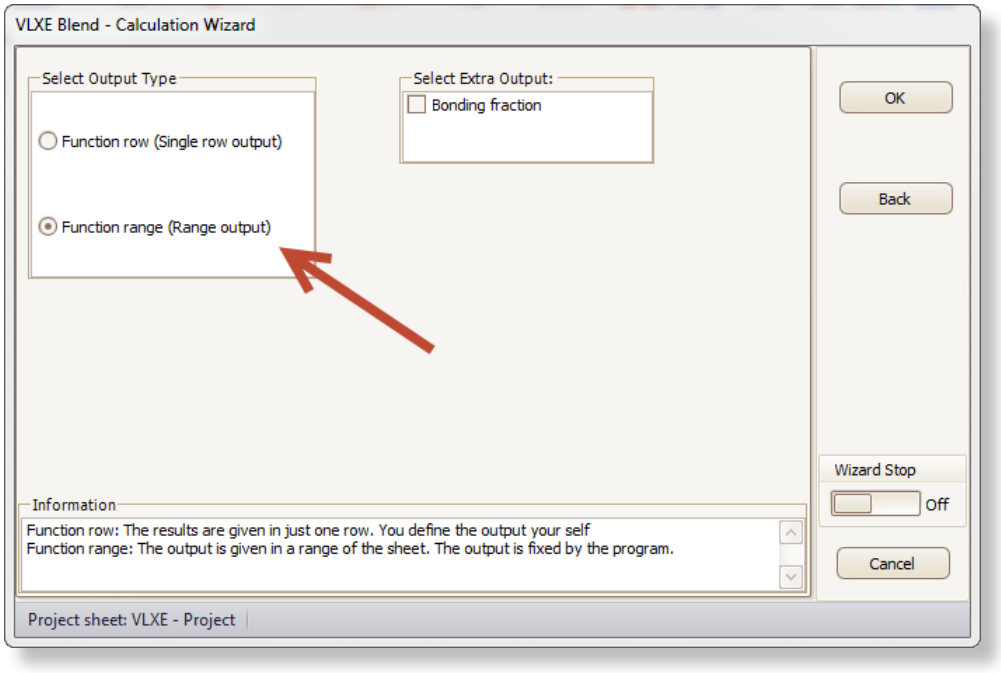
Go to a new empty Excel sheet and click on “Calculations” on the VLXE Blend ribbon. Leave the component list unchanged and click “Next”. Select “Cloud Point” and click “Next”.



Note that 2 new input options are provided. We can now chose point type and temperature range. Select "Auto" for range and "0 - 300" for temperature range. VLXE Blend will look for a solution within this range only.

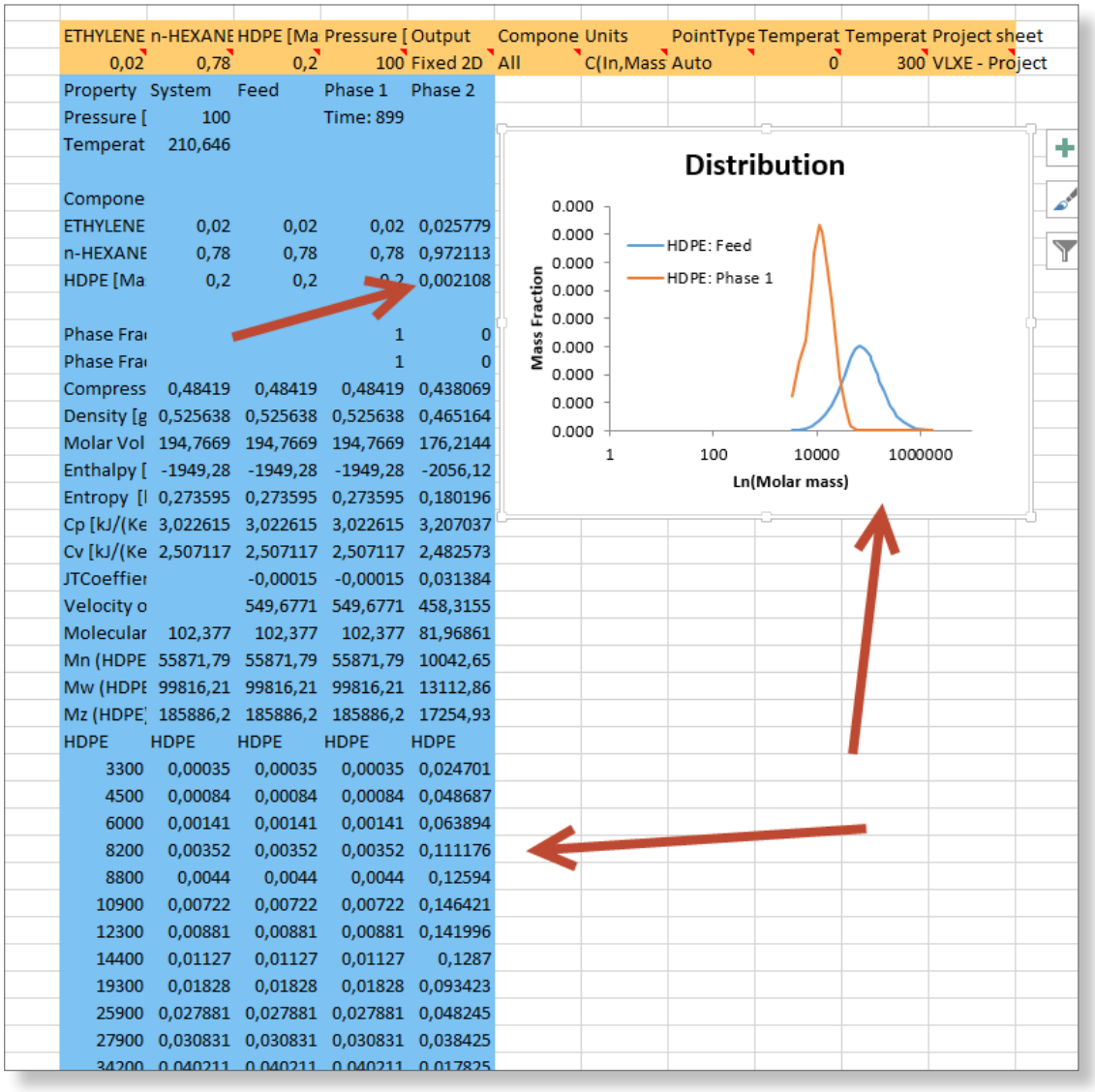


Under output, select "Function range" and leave "Bonding fraction" unchecked.



Select "OK" to create the calculation.
The output now includes distribution information but is otherwise the same as for "non-polymer" systems.

Note the distribution between the 2 phases , and also how there is 0.002 mass fraction in the second liquid phase. VLXE Blend not only finds the LLE system but will also give the distribution information.



ETHYLENE	n-HEXANE	HDPE [Ma	Pressure [	Output	Compone	Units	PointType	Temperat	Temperat	Project sheet
0,02	0,78	0,2	100	Fixed 2D	All	C(In,Mass	Auto	0	300	VLXE - Project

Property	System	Feed	Phase 1	Phase 2
Pressure [	100		Time: 899	
Temperat	210,646			
Compone				
ETHYLENE	0,02	0,02	0,02	0,025779
n-HEXANE	0,78	0,78	0,78	0,972113
HDPE [Ma	0,2	0,2	[illegible]	0,002108
Phase Frac			1	0
Phase Frac			1	0
Compress	0,48419	0,48419	0,48419	0,438069
Density [g	0,525638	0,525638	0,525638	0,465164
Molar Vol	194,7669	194,7669	194,7669	176,2144
Enthalpy [	-1949,28	-1949,28	-1949,28	-2056,12
Entropy [I	0,273595	0,273595	0,273595	0,180196
Cp [kJ/(Ke	3,022615	3,022615	3,022615	3,207037
Cv [kJ/(Ke	2,507117	2,507117	2,507117	2,482573
JTCoeffier		-0,00015	-0,00015	0,031384
Velocity o		549,6771	549,6771	458,3155
Molecular	102,377	102,377	102,377	81,96861
Mn (HDPE	55871,79	55871,79	55871,79	10042,65
Mw (HDPE	99816,21	99816,21	99816,21	13112,86
Mz (HDPE	185886,2	185886,2	185886,2	17254,93
HDPE	HDPE	HDPE	HDPE	HDPE
3300	0,00035	0,00035	0,00035	0,024701
4500	0,00084	0,00084	0,00084	0,048687
6000	0,00141	0,00141	0,00141	0,063894
8200	0,00352	0,00352	0,00352	0,111176
8800	0,0044	0,0044	0,0044	0,12594
10900	0,00722	0,00722	0,00722	0,146421
12300	0,00881	0,00881	0,00881	0,141996
14400	0,01127	0,01127	0,01127	0,1287
19300	0,01828	0,01828	0,01828	0,093423
25900	0,027881	0,027881	0,027881	0,048245
27900	0,030831	0,030831	0,030831	0,038425
34200	0,040211	0,040211	0,040211	0,017825

6.4 Flash Calculation

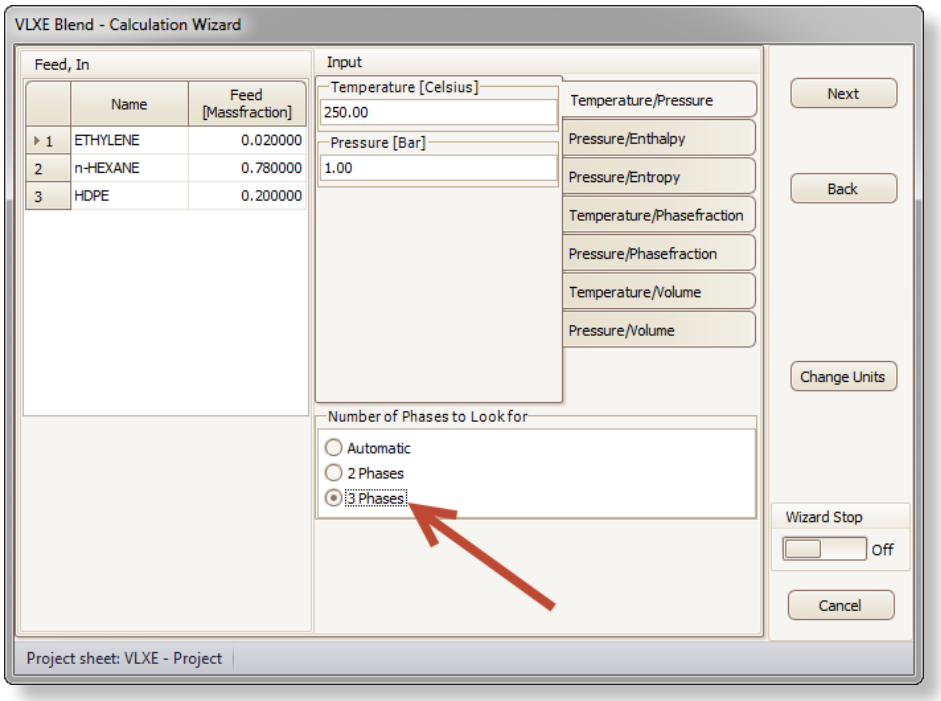
VLXE Blend offers the most commonly used flash calculations. They all automatically handle VLE or LLE. Not all can handle VLLE.

- Fixed Temperature & Pressure.
- Fixed Pressure & Enthalpy (Isenthalpic flash).
- Fixed Pressure & Entropy (isentropic flash).
- Fixed pressure and volume (2 phase flash only).
- Fixed temperature and volume (2 phase flash only).
- Fixed pressure and phase fraction (2 phase flash only).
- Fixed temperature and phase fraction (2 phase flash only).

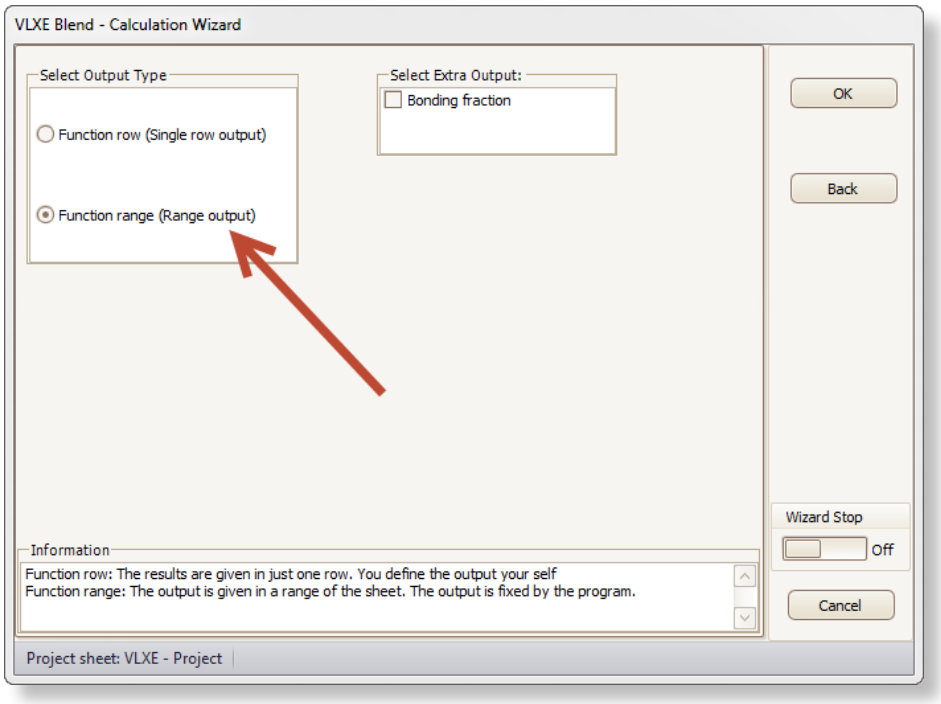
6.4.1 Flash at fixed temperature and pressure

We will now set up a flash calculation. VLXE Blend supports robust VLE, LLE and VLLE flash calculations for any polymer system. When we go through the steps in the calculation wizard, note how they are the same as for Methane + n-Hexane.

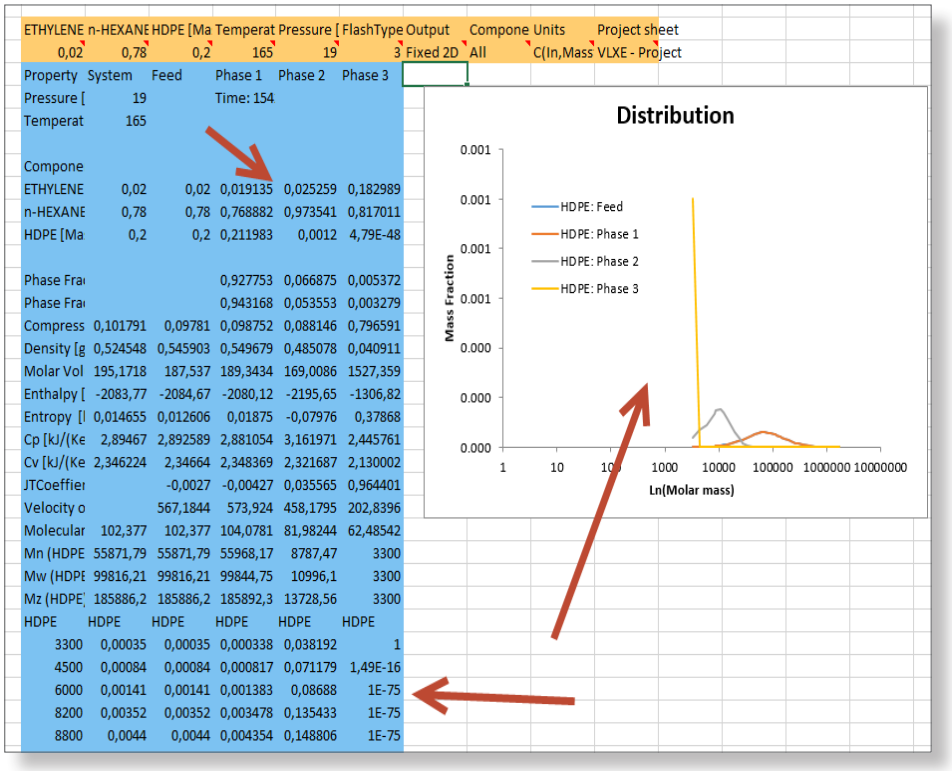
Go to a new empty sheet and click on “Calculations” on the VLXE Blend ribbon. Leave the component list unchanged and click “Next”. Select “Flash” and click “Next”. Note that there is no additional input for a polymer flash calculation. Select “3 Phase” flash and select “Next”



Select “Function range” as output and select “OK” to create the calculation



Adjust temperature to 165ºC and pressure to 19 Bar. Note how VLXE Blend finds a VLLE system and how the polymer distributes between the 3 phases.



ETHYLENE	n-HEXANE	HDPE [Ma	Temperat	Pressure [	FlashType	Output	Compone	Units	Project sheet
0,02	0,78	0,2	165	19	3	Fixed 2D	All	C(In,Mass	VLXE - Project

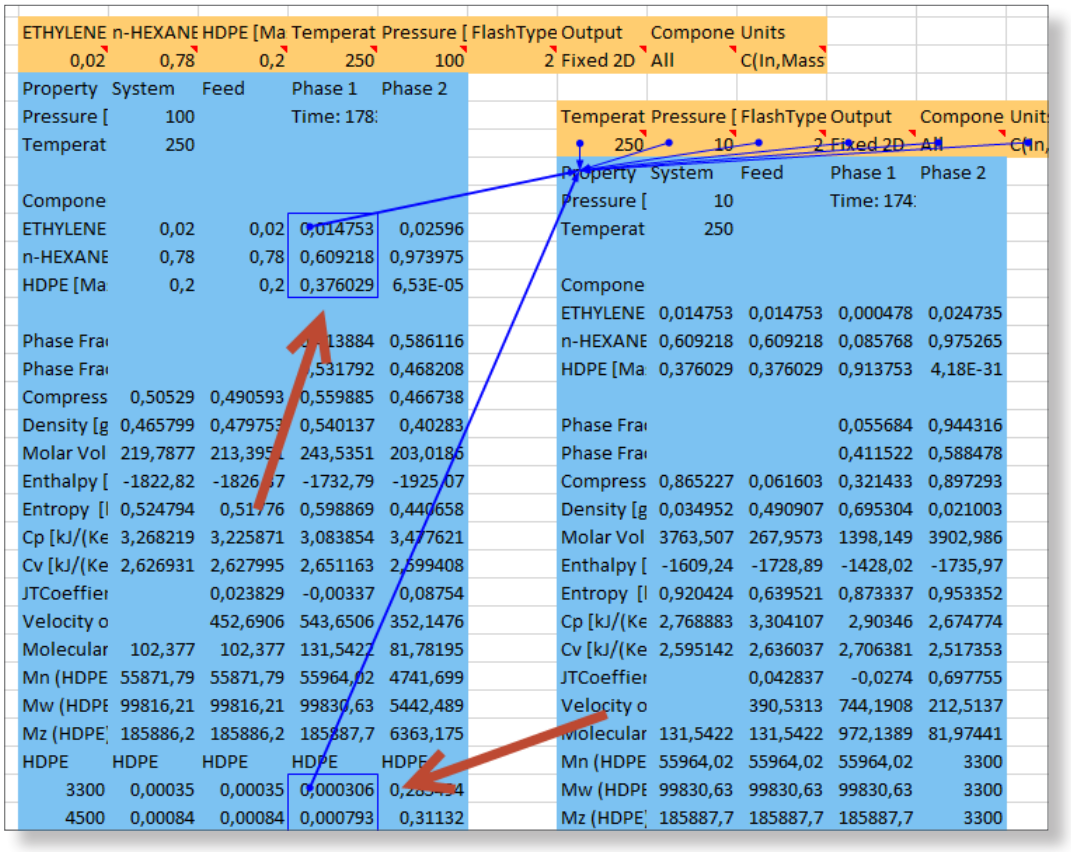
Property	System	Feed	Phase 1	Phase 2	Phase 3
Pressure [	19		Time: 154		
Temperat	165				
Compone					
ETHYLENE	0,02	0,02	0,019135	0,025259	0,182989
n-HEXANE	0,78	0,78	0,768882	0,973541	0,817011
HDPE [Ma	0,2	0,2	0,211983	0,0012	4,79E-48
Phase Frac			0,927753	0,066875	0,005372
Phase Frac			0,943168	0,053553	0,003279
Compress	0,101791	0,09781	0,098752	0,088146	0,796591
Density [g	0,524548	0,545903	0,549679	0,485078	0,040911
Molar Vol	195,1718	187,537	189,3434	169,0086	1527,359
Enthalpy [	-2083,77	-2084,67	-2080,12	-2195,65	-1306,82
Entropy [I	0,014655	0,012606	0,01875	-0,07976	0,37868
Cp [kJ/(Ke	2,89467	2,892589	2,881054	3,161971	2,445761
Cv [kJ/(Ke	2,346224	2,34664	2,348369	2,321687	2,130002
JTCoeffier		-0,0027	-0,00427	0,035565	0,964401
Velocity o		567,1844	573,924	458,1795	202,8396
Molecular	102,377	102,377	104,0781	81,98244	62,48542
Mn (HDPE	55871,79	55871,79	55968,17	8787,47	3300
Mw (HDPE	99816,21	99816,21	99844,75	10996,1	3300
Mz (HDPE	185886,2	185886,2	185892,3	13728,56	3300
HDPE	HDPE	HDPE	HDPE	HDPE	HDPE
3300	0,00035	0,00035	0,000338	0,038192	1
4500	0,00084	0,00084	0,000817	0,071179	1,49E-16
6000	0,00141	0,00141	0,001383	0,08688	1E-75
8200	0,00352	0,00352	0,003478	0,135433	1E-75
8800	0,0044	0,0044	0,004354	0,148806	1E-75

6.4.2 Link Flash Calculation

Linking two or more flash calculations allows you to simulate a separation unit in Excel. For poly-disperse polymers the distribution will change between units since the pseudo-components will not distribute equally between the phases in the separator. VLXE Blend supports this in a very simple manner. Simply overwrite the distribution that a calculation is to use by passing it a new one using the “Distribution” argument.

As an example we will now link 2 flash calculations where we feed the heavy phase from the first flash into the second flash. This can be seen as 2 separators in series.

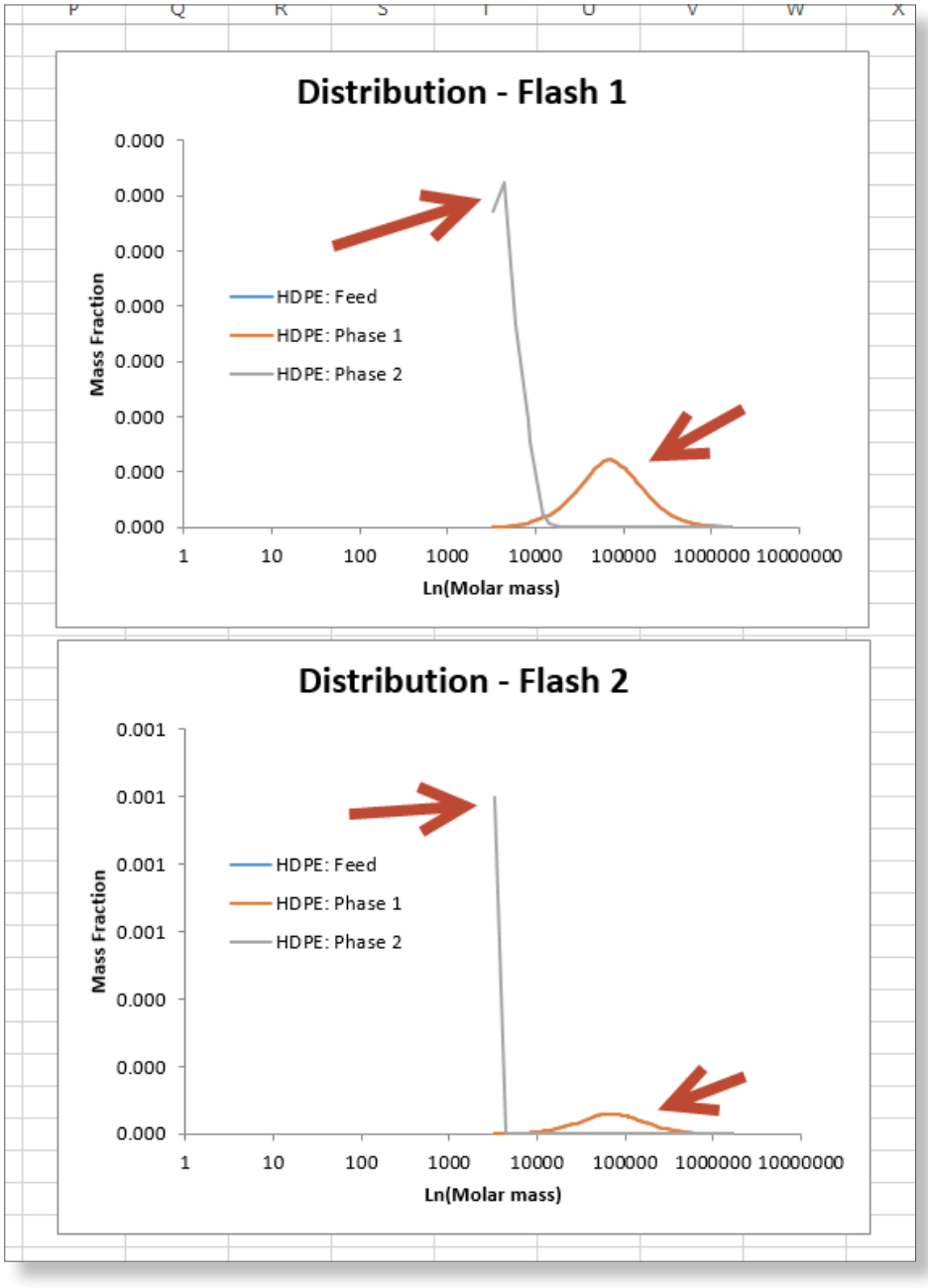
Use the wizard and create 2 flash calculations as shown below.



In the example above, Excel’s “Trace Dependents“ is activated. It visualises the links that a function is using.

Note how the second flash gets its feed and distribution from the result in the first flash. Also note how the polymer content of the phases changes. The second flash units has virtually no polymer in the vapor phase, while the first flash does.

The distribution for the 2 flash units is shown below. Note how the feed changes for the second flash.



6.5 Phase Diagram

VLXE Blend provides a method to map out the entire phase envelope, including the VLE, LLE, VLLE and SLE regions. In addition to this, lines of fixed properties can be traced in the phase diagram. In other words, a complete picture of the phase diagram can be obtained.

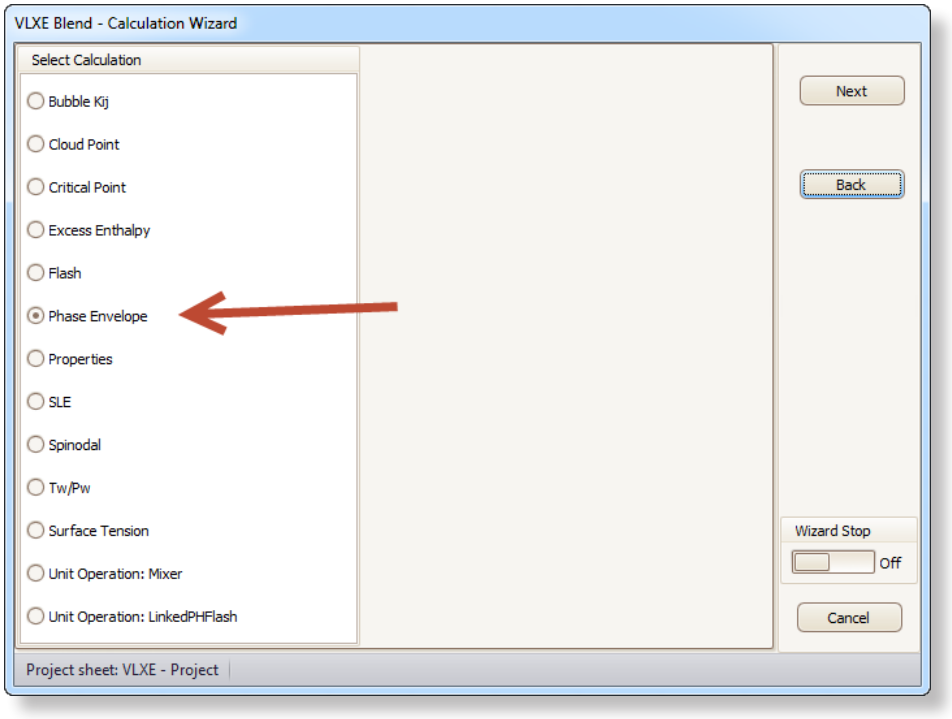
Phase envelope can be viewed in three different ways:

- Ordinary phase envelope.
- Polymer mass fraction versus Temperature (Tw).
- Polymer mass fraction versus Pressure (Pw).

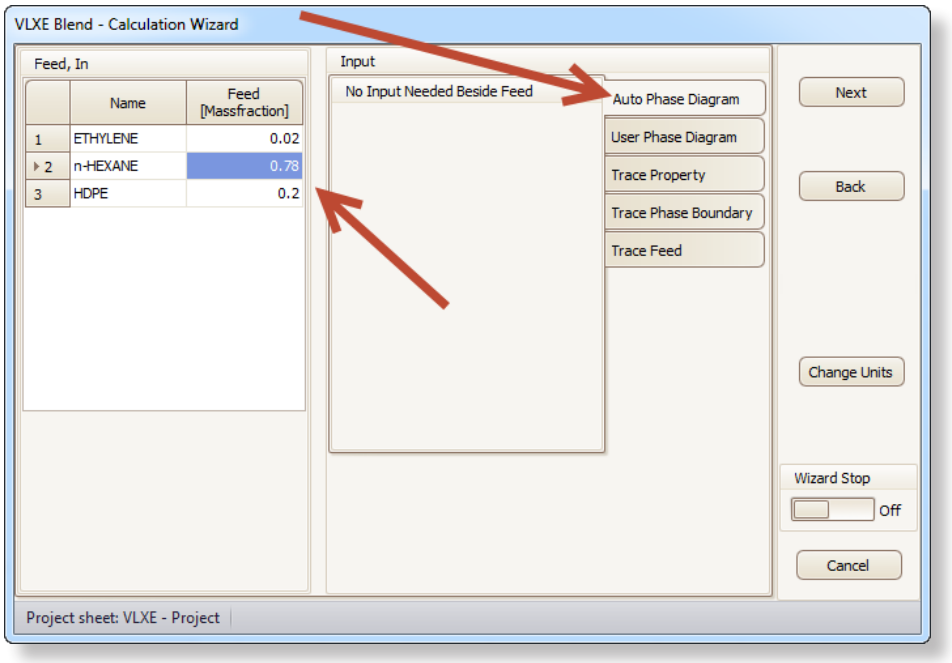
6.5.1 Phase Envelope including VLLE region

To illustrate the robustness of the routines in VLXE Blend we will map the entire phase diagram for the previous polymer system, including the VLLE area. The routine cannot get this in one call, so you have to make 2 calculations and then combine the plots.

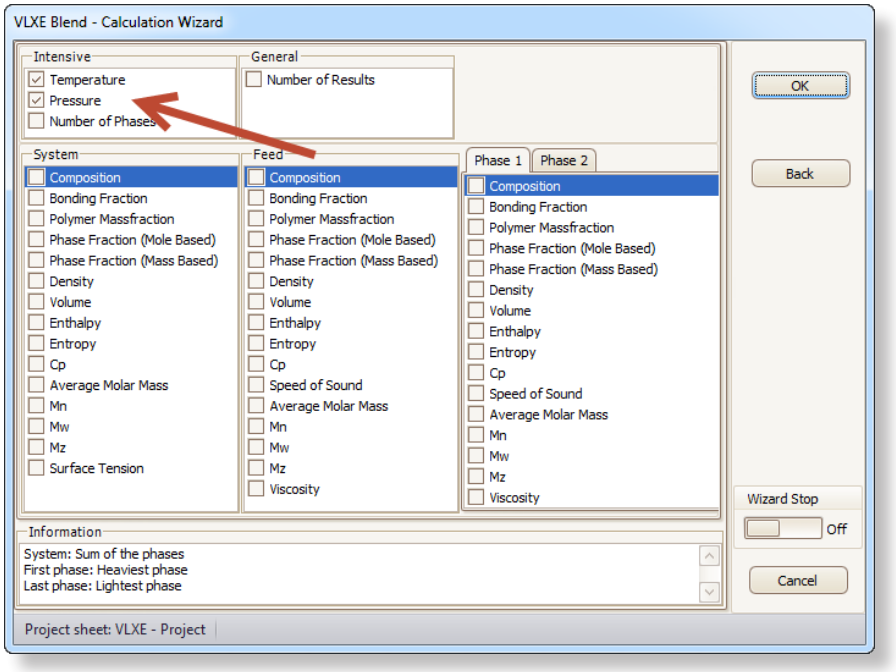
Start by selecting “Calculations” on the VLXE Blend ribbon. Click “Next” on the first page leaving in all 3 components. Select “Phase envelope” then “Next”.



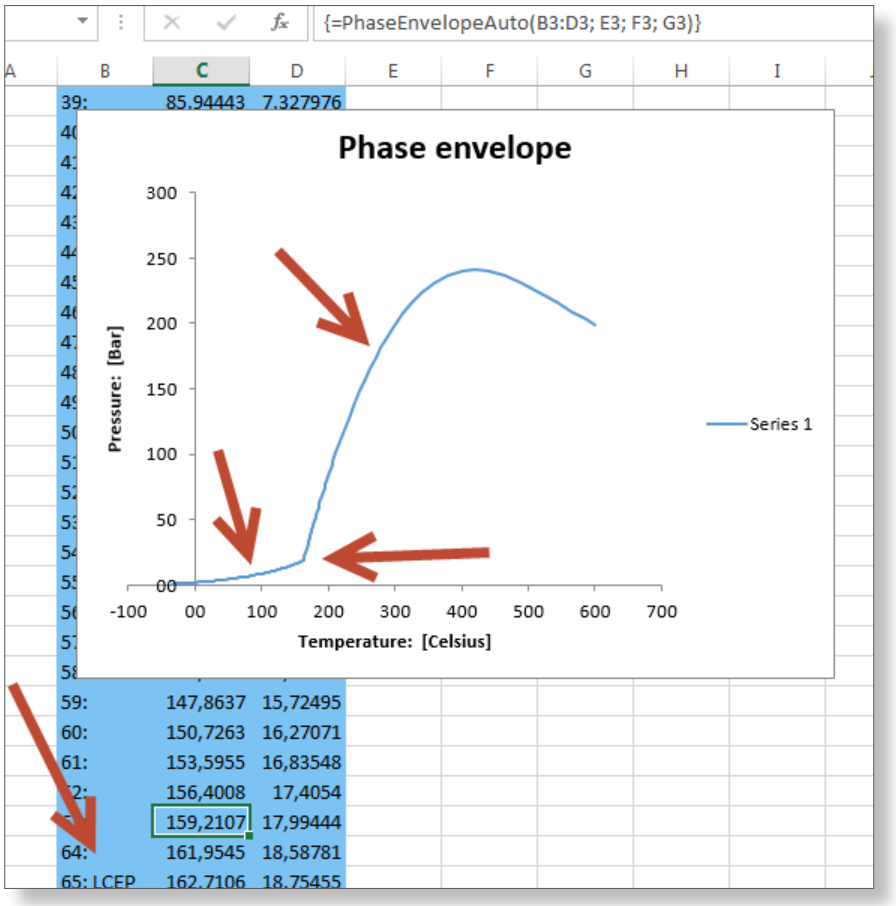
Select “Auto Phase Diagram” and then “Next”.



Leave the output part unchanged. For this type of calculation, temperatue and pressure is preselected.



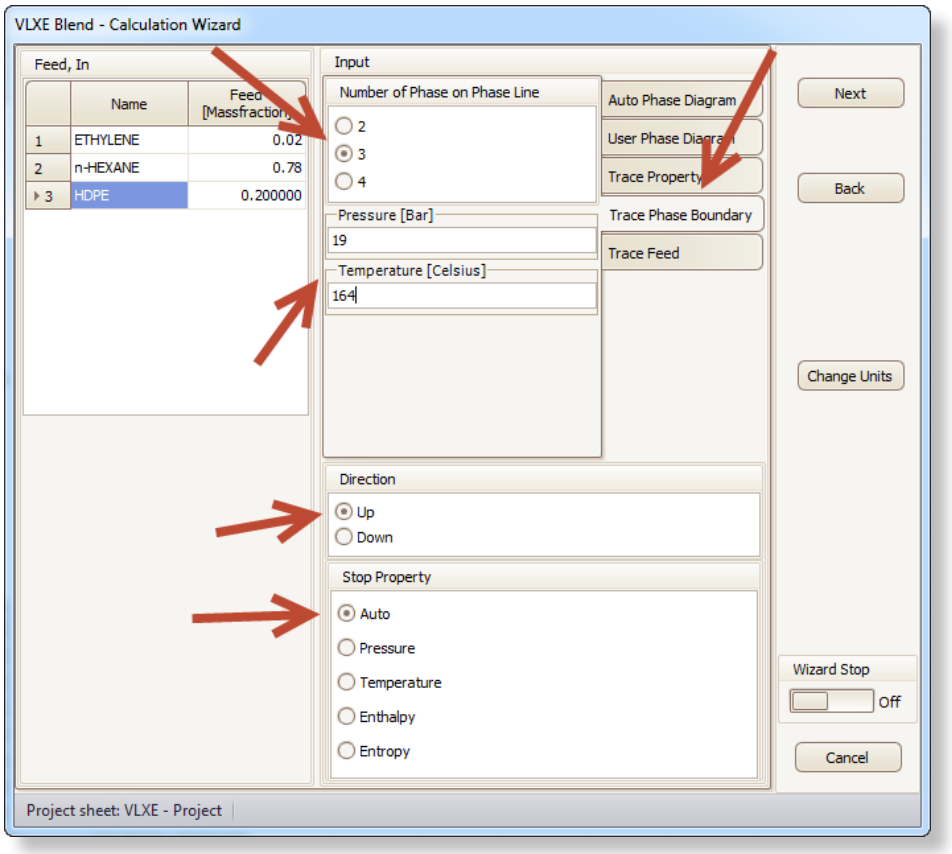
Now select “OK” to generate the calculation.



Note how VLXE Blend captures the entire 2 phase area including the VLE and LLE lines. Plus it finds the LCEP where the 2 lines meet. PC-SAFT will trace the entire phase diagram. But since polymers decompose at higher temperatures, the built in stopping point is set to 600°C.

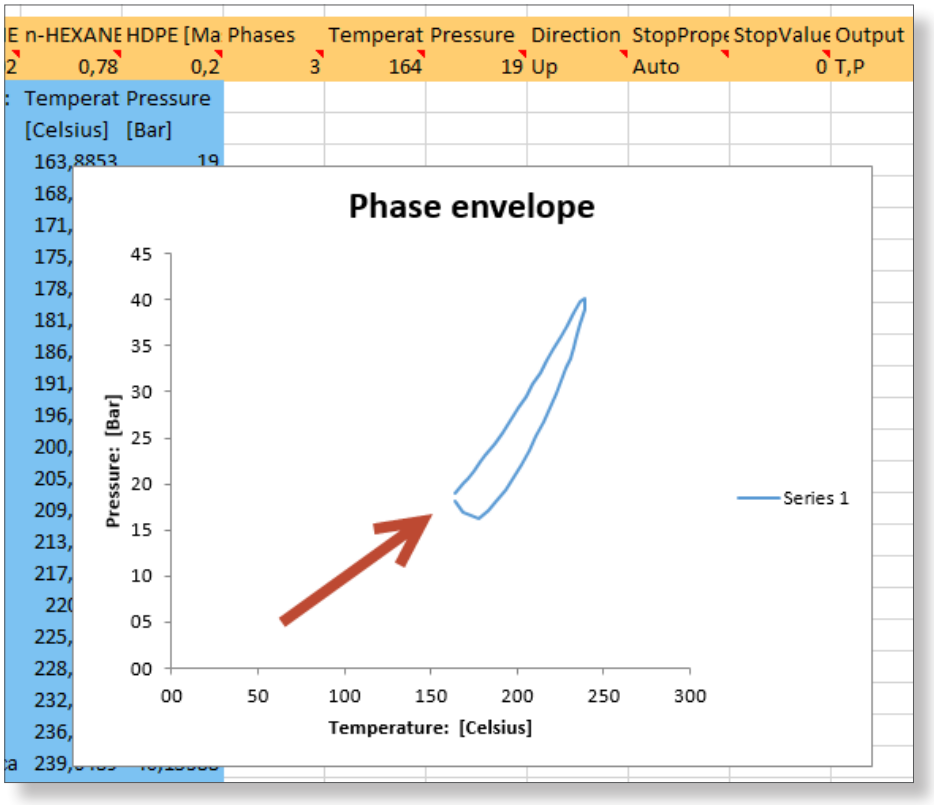
Now we want to find the VLLE area. We know it starts at the LCEP so we will use that information as an initial guess to start the routine that will calculate the VLLE line.

The LCEP is at 163°C and 19 Bar. Make a note of that and then select "Calculation" on the VLXE ribbon. Again select "Phase diagram" as the calculation type and select "Next". Now select "Trace Phase Boundary" and make the selection as given below. The starting point needs to be inside the 3-phase area and close to the phase boundary.

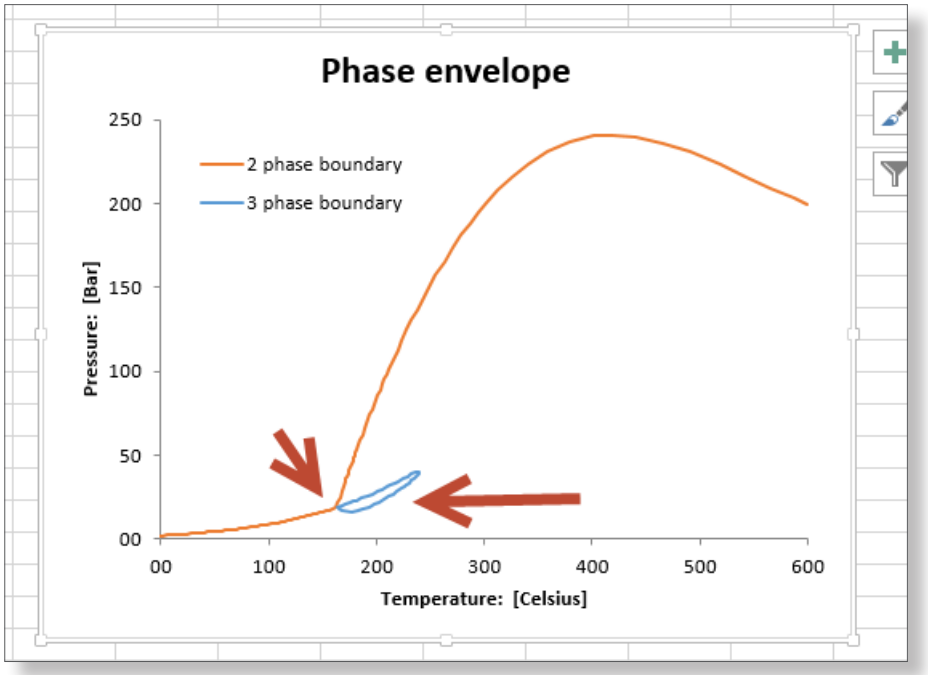


Select "Next" and under output select "OK" to generate the calculation.

The result is the phase boundary for the VLLE area.



Now merge the 2 charts to get the entire phase diagram. In Excel this can be done by Copy/Paste. The result is shown below:

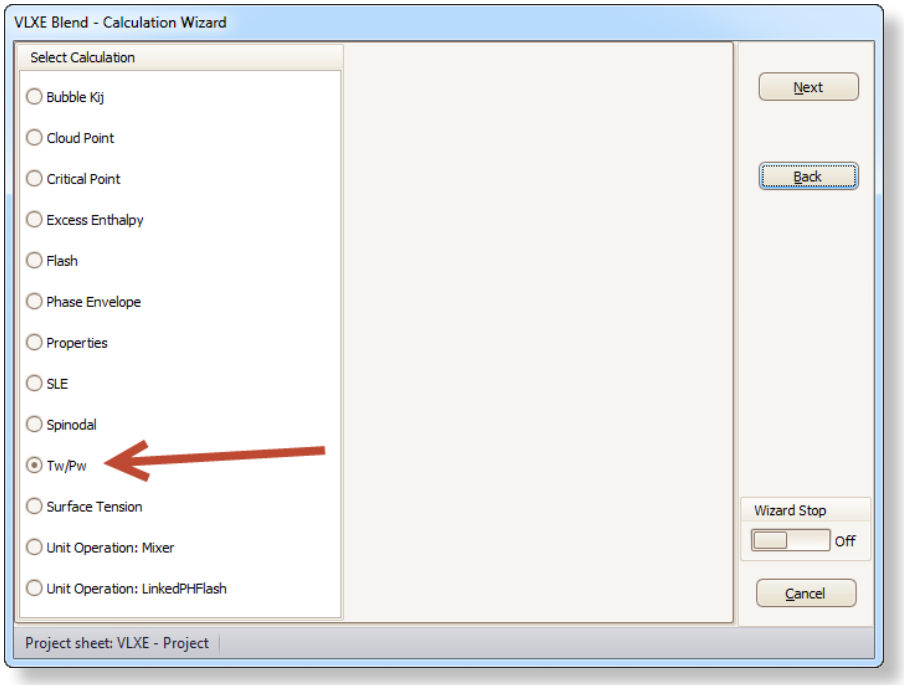


Knowing the entire phase diagram is very important when performing process simulations. In the separation steps the 3-phase area is to be avoided, and looking at the chart above it can be seen that for this system the VLLE area is right on the separation path. The phase diagram above has been verifyed by experimental data and currently an HDPE producing company is using it to plan their separation process.

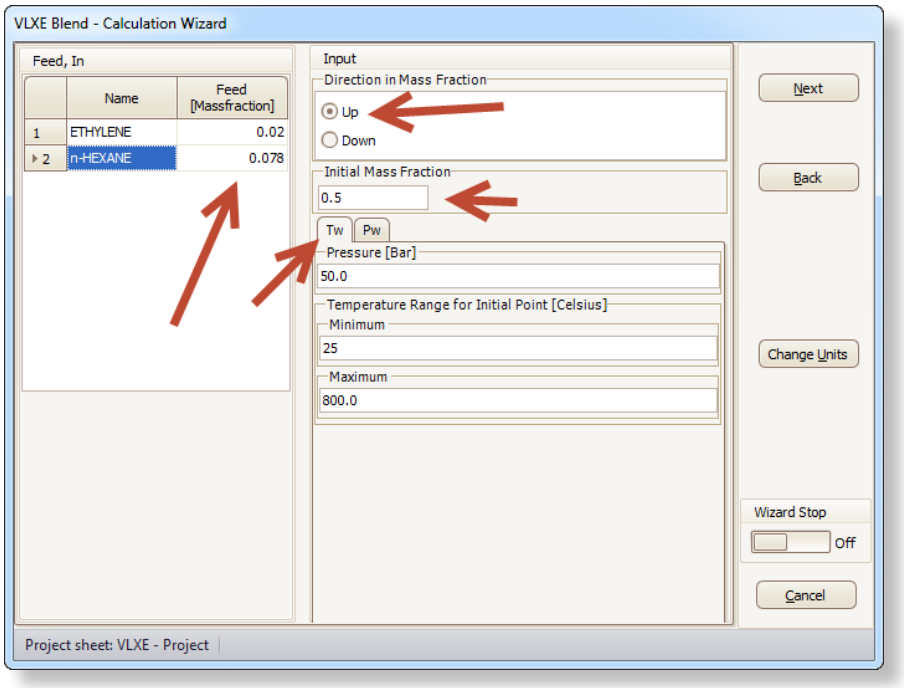
6.6 Polymer Mass Fraction vs Temperature (wT)

We have just plotted the entire phase envelope in the temperature vs. pressure space. If you imagine the polymer mass fraction of the mixture as the 3rd dimension, you get a temperature, pressure, polymer mass fraction (w) cube. The phase envelope is a "slice" of this cube in the temperature and pressure space. Now we will work with the 2 other possible slides, wT and wP.

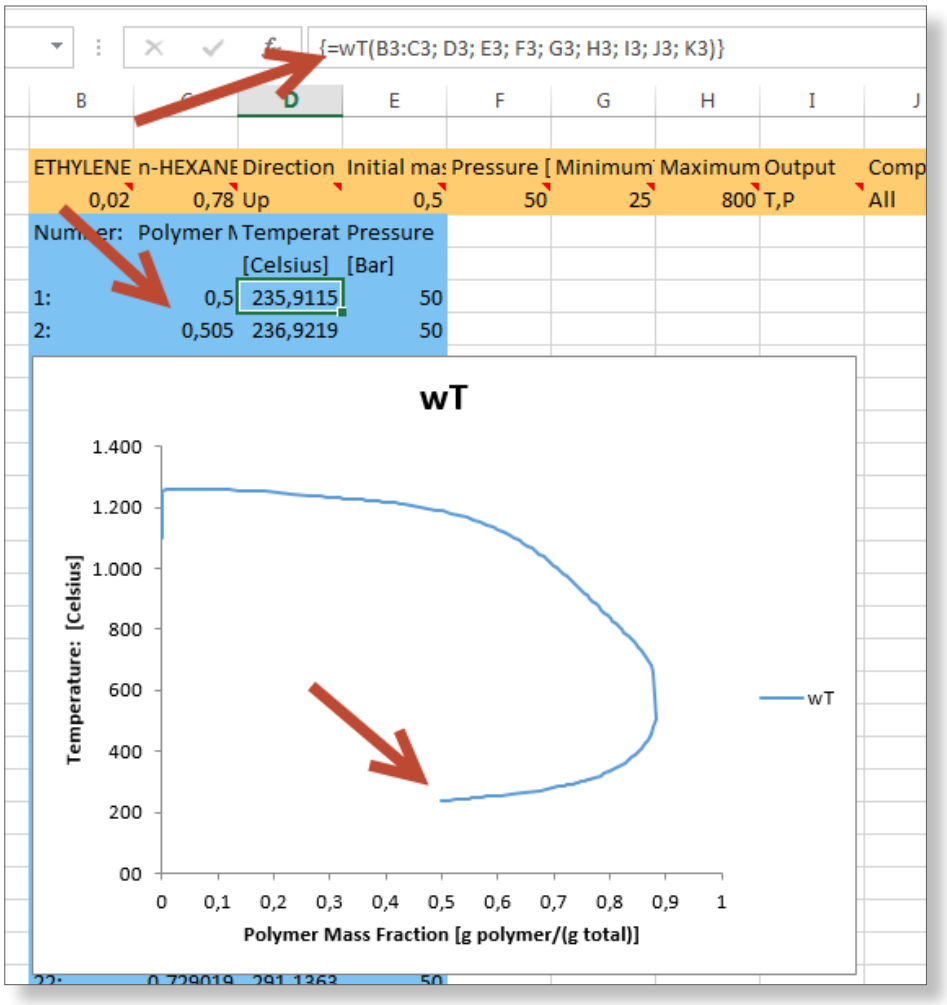
First we will create a polymer mass fraction vs. temperature plot, from now on referred to as wT. In order to cover polymer mass fraction from 0 to 1 we have to generate 2 curves.
Select "Calculation" on the VLXE blend ribbon. Go to the page where the calculation is selected and click on "wT/wP".



Select "Next" and set the input as given below.



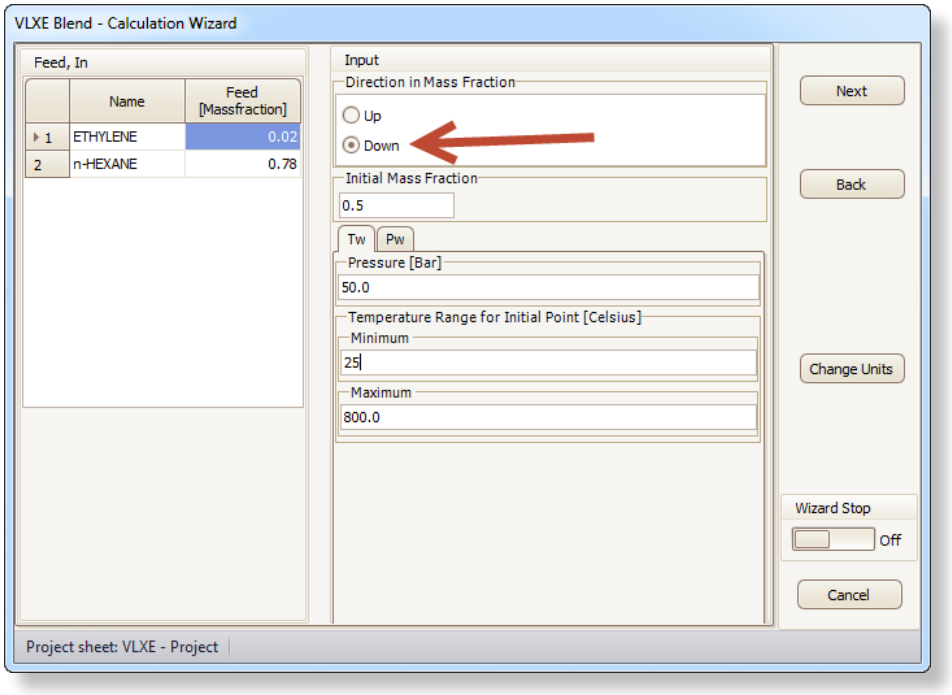
Note how only the solvent composition is required now. The other settings mean that the curve will start at a polymer mass fraction of 0.5 and then trace the phase boundary as a function of polymer mass fraction and temperature at a fixed pressure of 50 Bar.



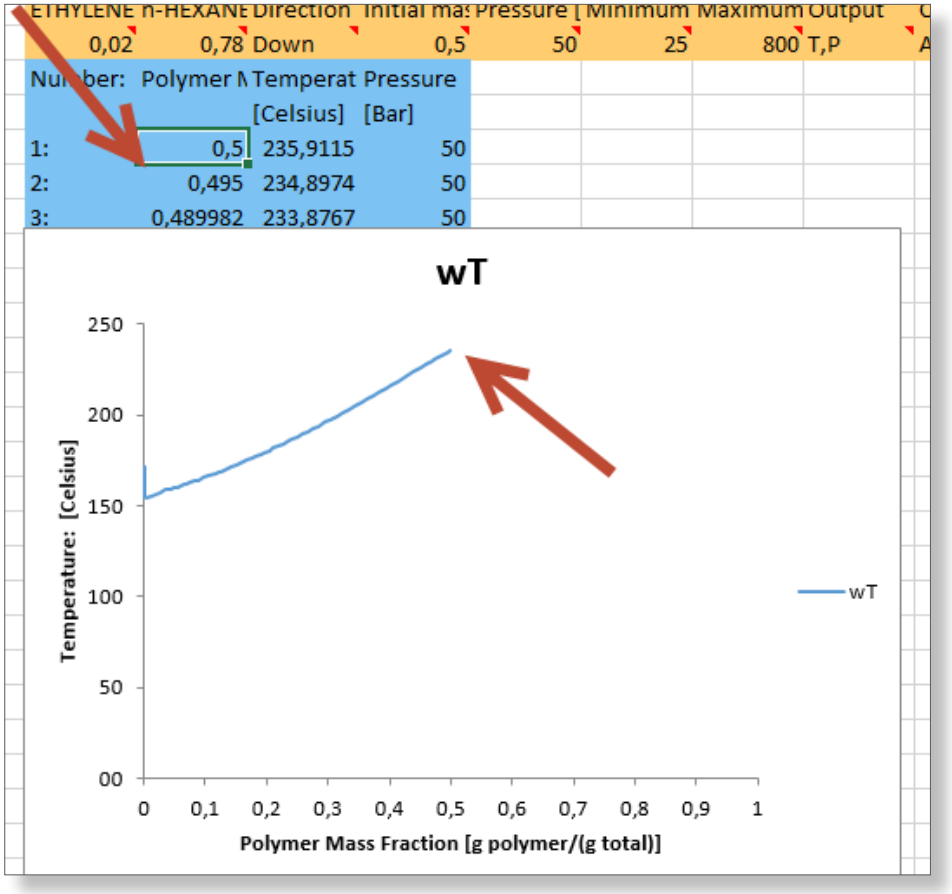
Note how the curve starts at a polymer mass fraction of 0.5 and then follows the phase boundary as far as it can. PC-SAFT will model the entire curve even though it goes beyond the boundary of temperatures which are physically possible.

On the inside of the curve is the 2 phase area, and outside is the 1 phase.

In a similar way we will now repeat the calculation, only now we will go down in polymer mass fraction.

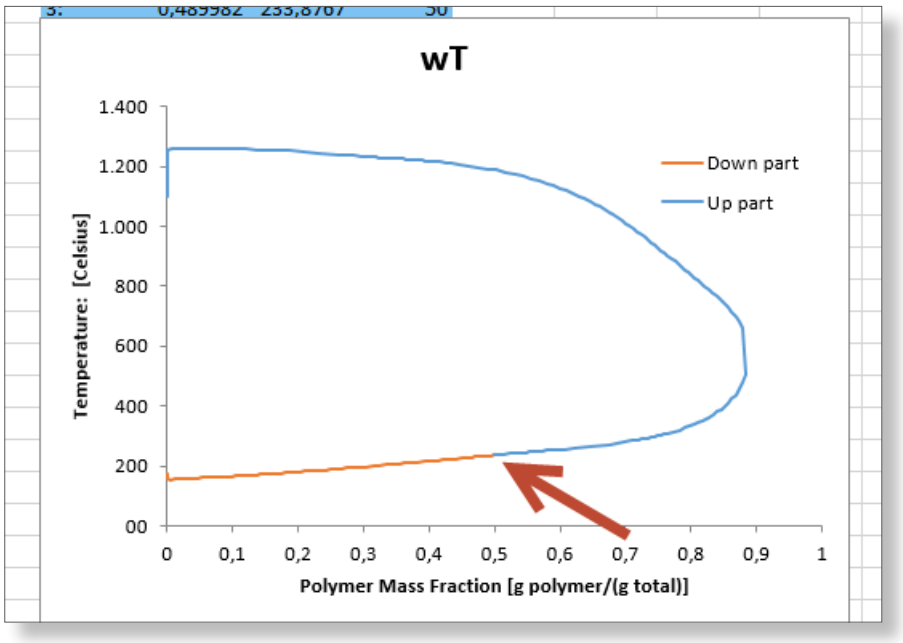


Using the default output to generate the calculation, select “Next” and then “OK”.



Note how the curve now starts at a polymer mass fraction of 0.5 and then follows the phase boundary down to 0 polymer mass fraction.

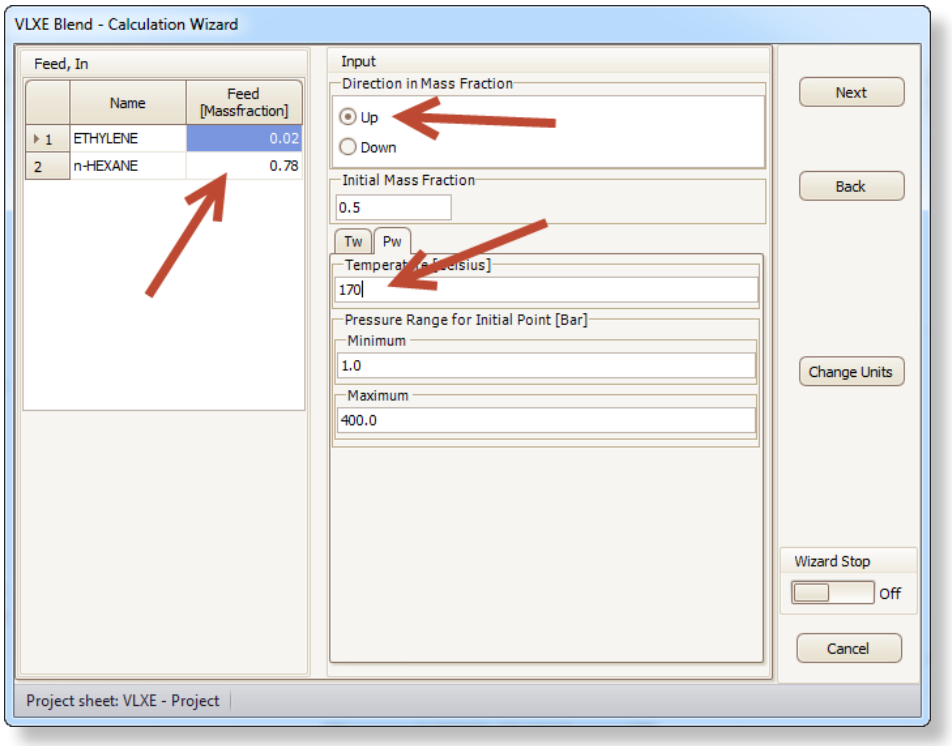
Now combine the 2 charts to get the entire phase boundary at 50 Bar.



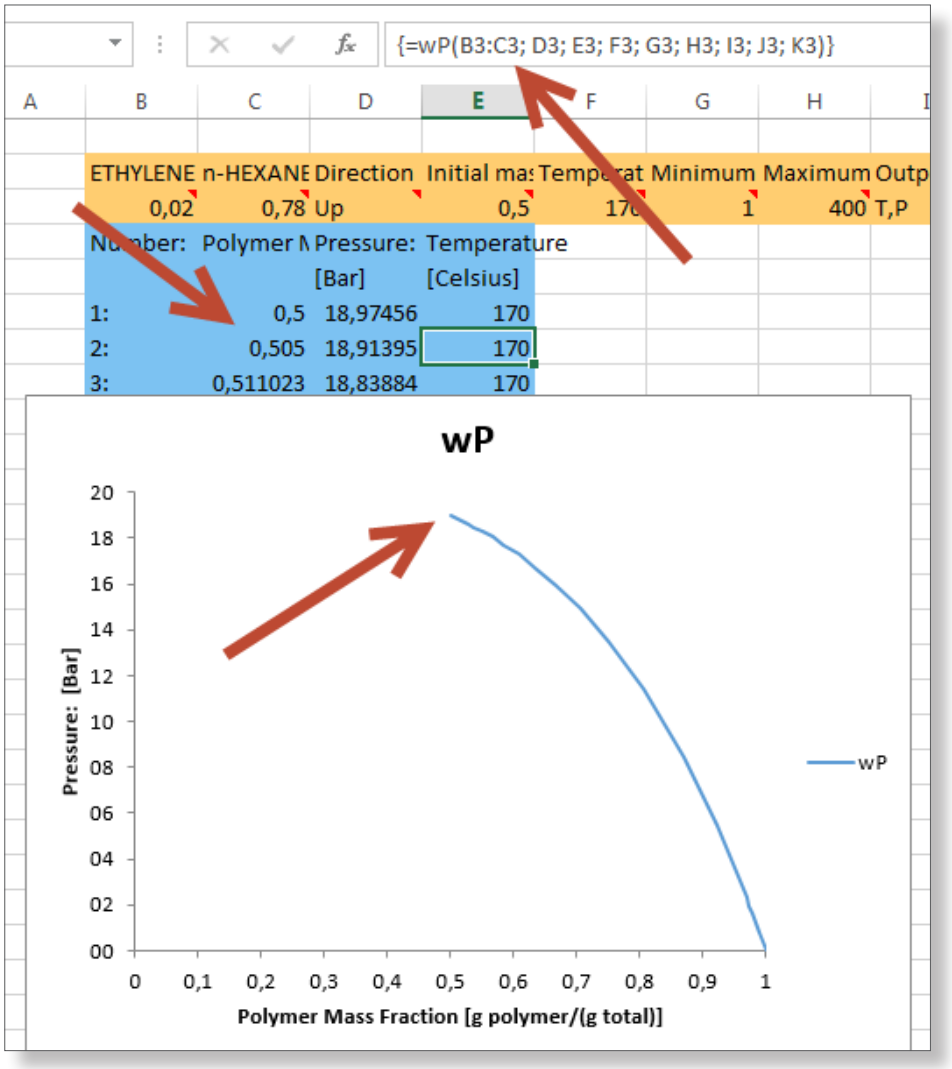
The result shows how this mixture behaves at 50 Bar for a fixed ratio of solvents. Inside the curve is the 2 phase area and outside is the 1 phase.

6.7 Polymer Mass Fraction vs Pressure (wP)

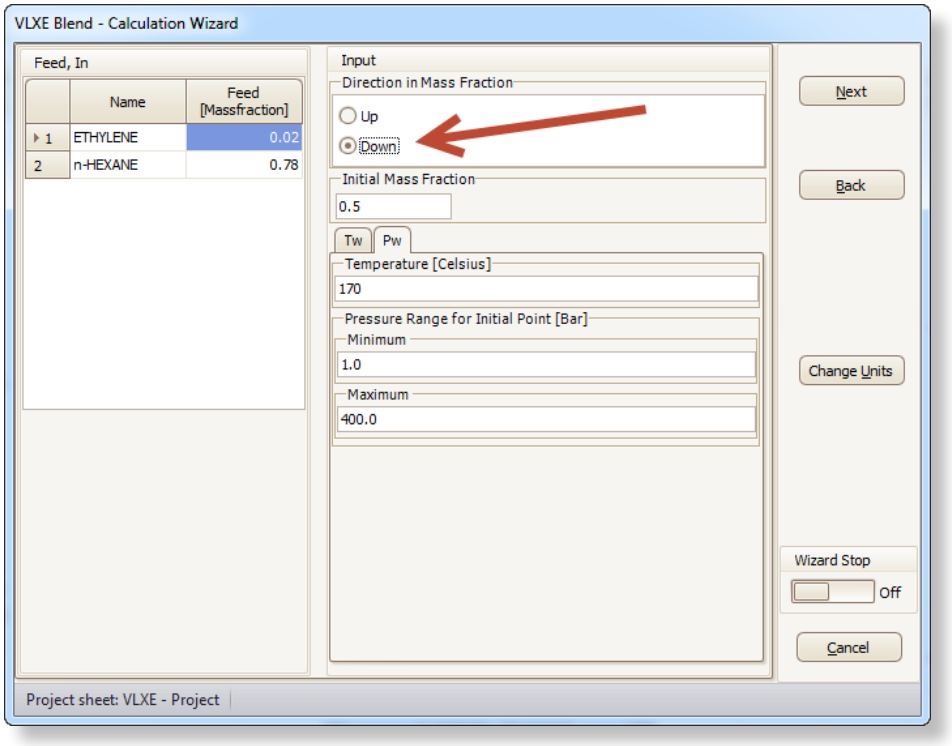
The wP plot is generated just as for the wT plot. Select “Calculation” on the VLXE Blend ribbon. Select “wT/wP” as calculation and click on “Next”. Set the input as shown below:



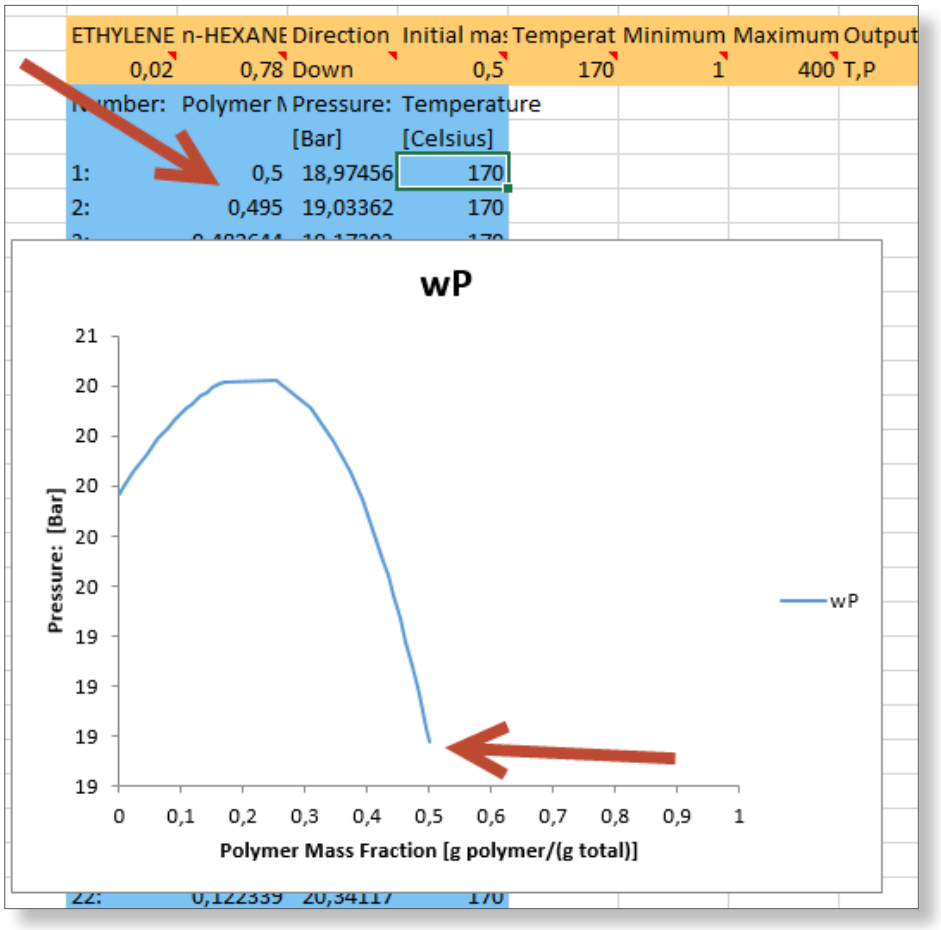
Using the default output, select “Next” and then “OK”.
The calculation is now created.



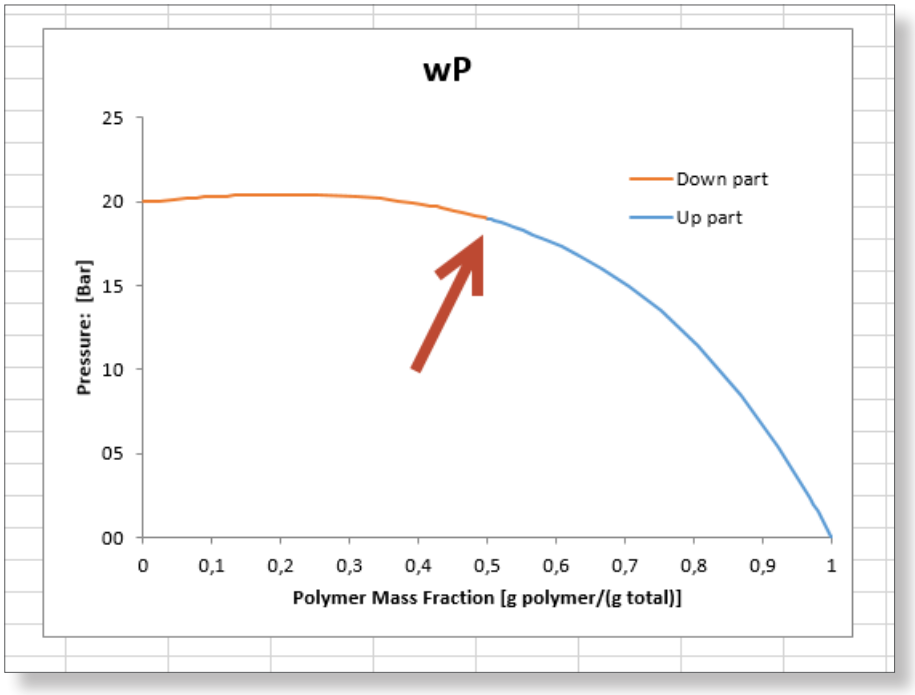
In order to get the last part of the curve we repeat, the only change is that we now select “Down” as direction.



Again, select “Next” and then “OK” to generate the calculation.



Now combine the 2 plots to get the entire phase boundary.



Below the curve is the 2 phase area and above the 1 phase area. Try to verify with the phase envelope that the 2 curves meet at the right place. Keep in mind that the 2 curves are just 2 different slices of the same temperature, pressure, polymer mass fraction cube.

6.8 SLE

In this section we provide a description of Solid-Liquid calculations (SLE). It´s an imperative calculation for systems containing polymers, since solid polymer is the end product. Here an assumption is made for SLE calculations, that being that the solid phase does not contain any solvent. When performing SLE calculations the thermodynamic model is not the same for the different phases. Liquid and vapor phases are modeled by using an equation of state (EOS) and the solid phase is modeled by using a separate model that can only be used for solid phases.

Two different versions of the same model are implemented:

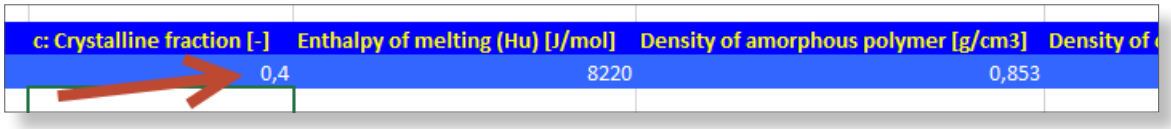
- Original Pan & Radosz
- Full Pan & Radoz

Here the original Pan & Radoz model is used (For details see VLXE Blend Help)

VLXE Blend provides the following options for SLE calculations:

- Temperature
- Polymer Mass Fraction
- T/P Curve
- PMF/T Curve

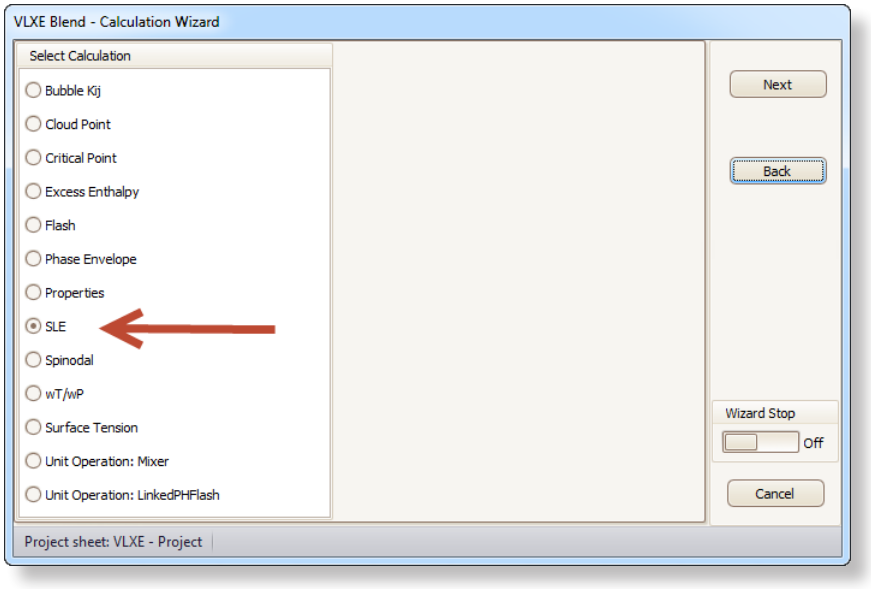
SLE calculations need parameters which are used only for these calculations. They can be seen in the project sheet. The values used in these examples are shown below. Note the crystalline fraction.



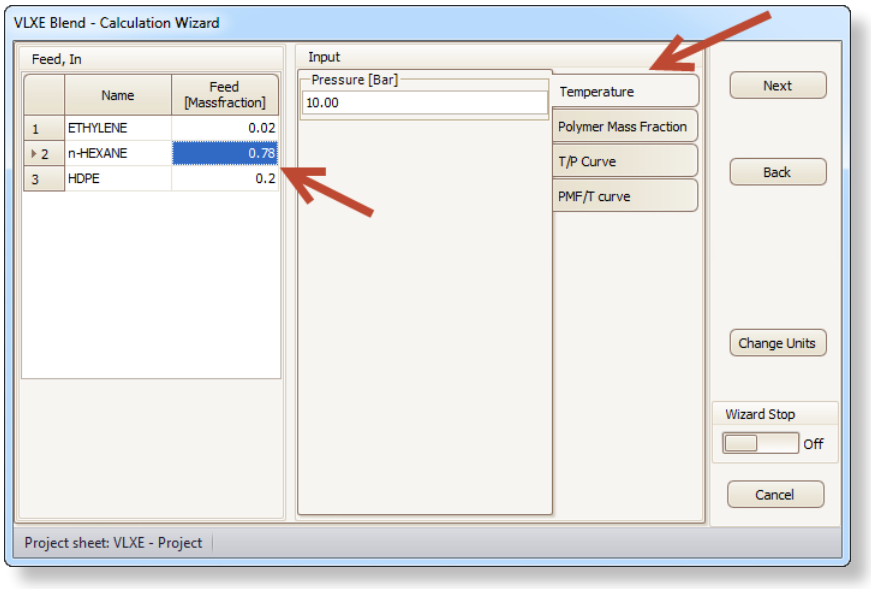
6.8.1 Temperature

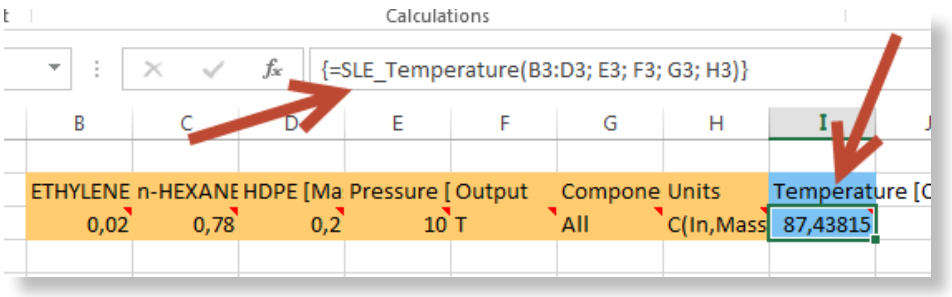
This calculation will find the SLE temperature for a given pressure and composition. That is the temperature where the solid phase forms. This is important process information since solid deposition inside the plant is to be avoided.

Select “Calculation” on the VLXE Blend ribbon. Leave all components in and select “SLE” as the calculation type. Select “Next”.



Select “Temperature” as the SLE calculation type, add feed and then select “Next”. Then “Next” to get row output format and then “OK” for default output.



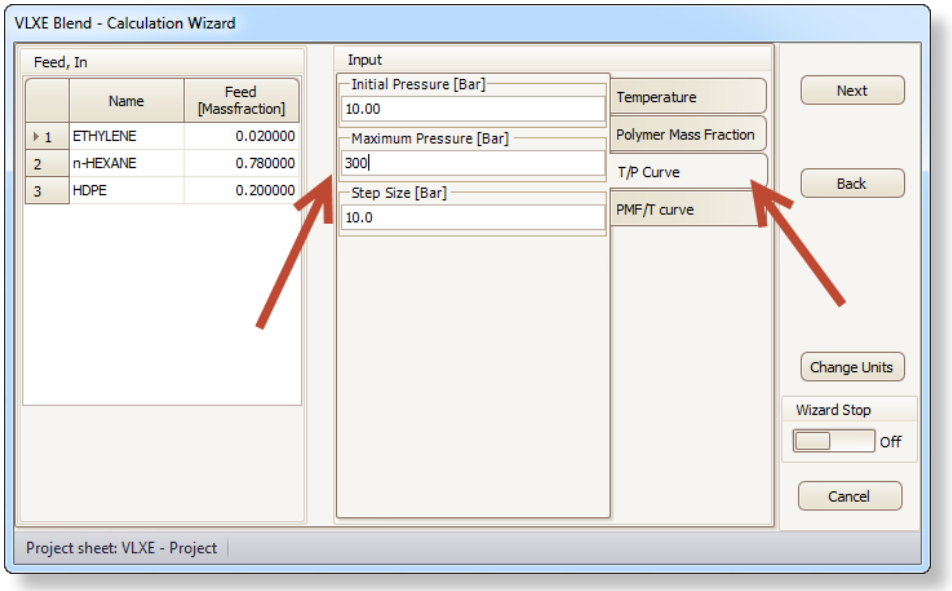


The calculation is then created. Note that below 87.4°C a solid phase will form for this system.

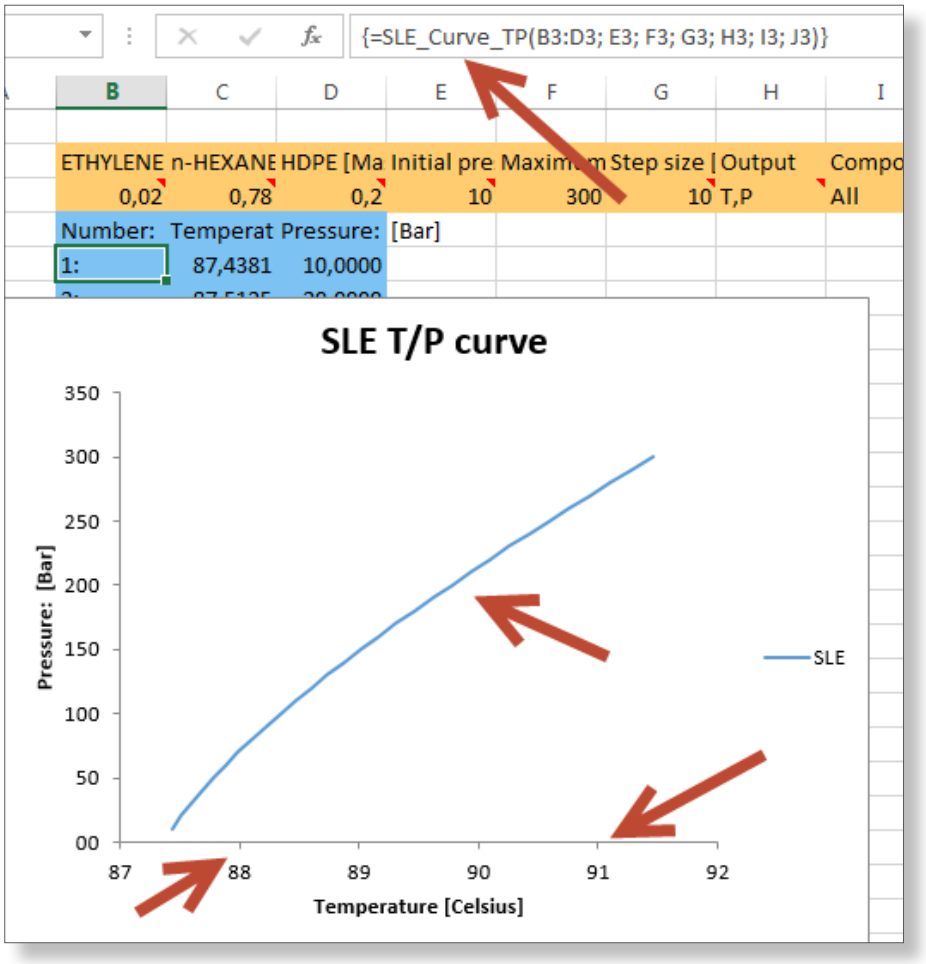
6.8.2 Temperature/Pressure Curve

The temperature/pressure (T/P) curve will calculate the phase boundary between solid forming and not forming. Together with the phase envelope it gives a very clear picture that can be used in process design.

Select “Calculation” on the VLXE Blend ribbon, select SLE and then “Next”.

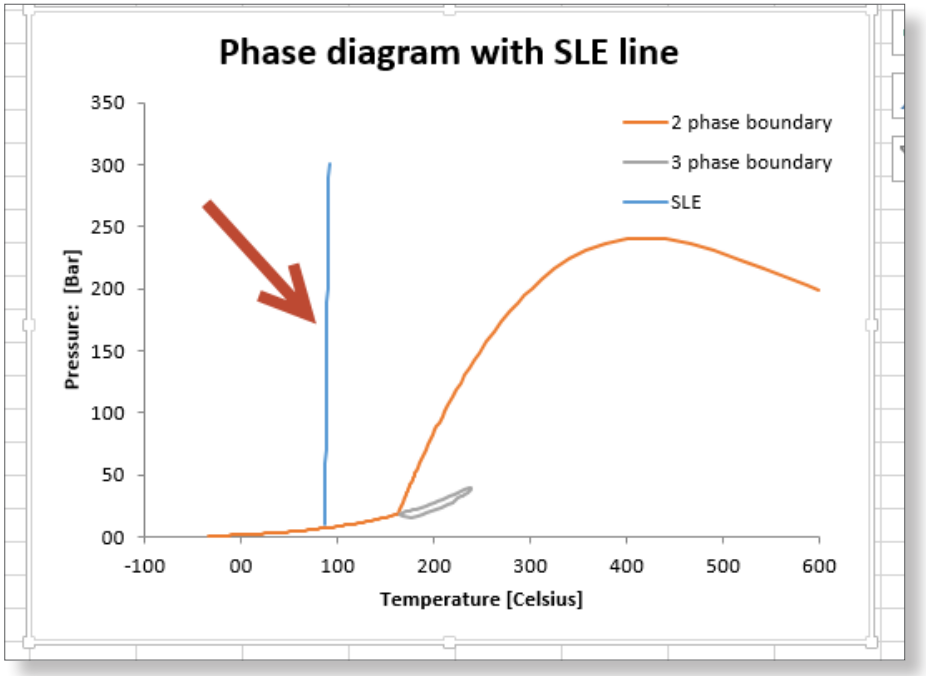


Select “T/P Curve” and set the input as given above. Then select “Next” and then “OK” using the default output. The calculation is now created.



Note the temperature range. The line is very vertical.

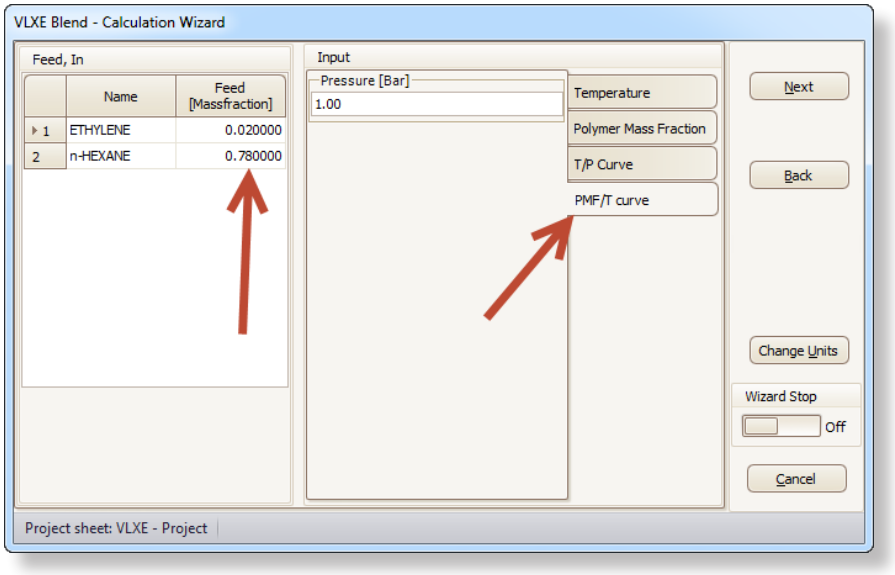
Now combine this plot with the phase diagram we made before.
The phase diagram is now complete with SLE information. For this mixture the SLE, VLE, LLE and VLLE region has now been defined, thereby facilitating process decisions to be made safely.



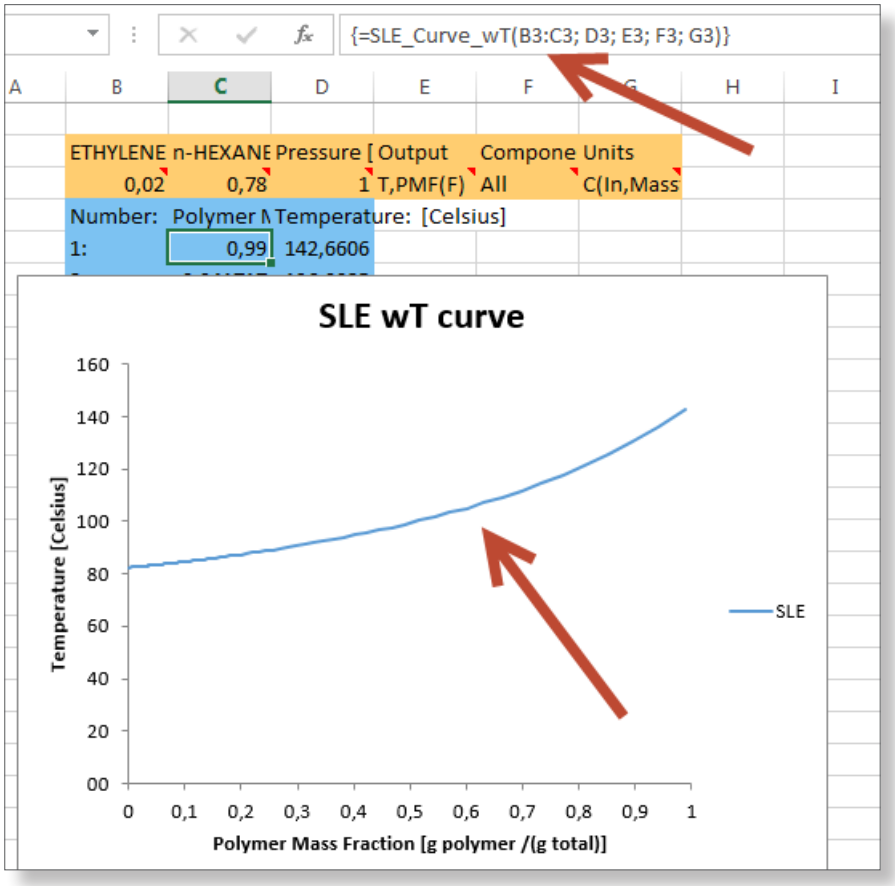
6.8.3 PMF/T Curve

This calculation lets the user fix pressure and obtain the phase boundary as a function of polymer mass fraction (PMF) and pressure. It is similar to what was done earlier for the wT and wP curves, except that we now look for SLE phase boundaries.

To set up this calculation, go again to the SLE calculation page in the wizard and make the selections as indicated below. Then create the calculation using the default output.



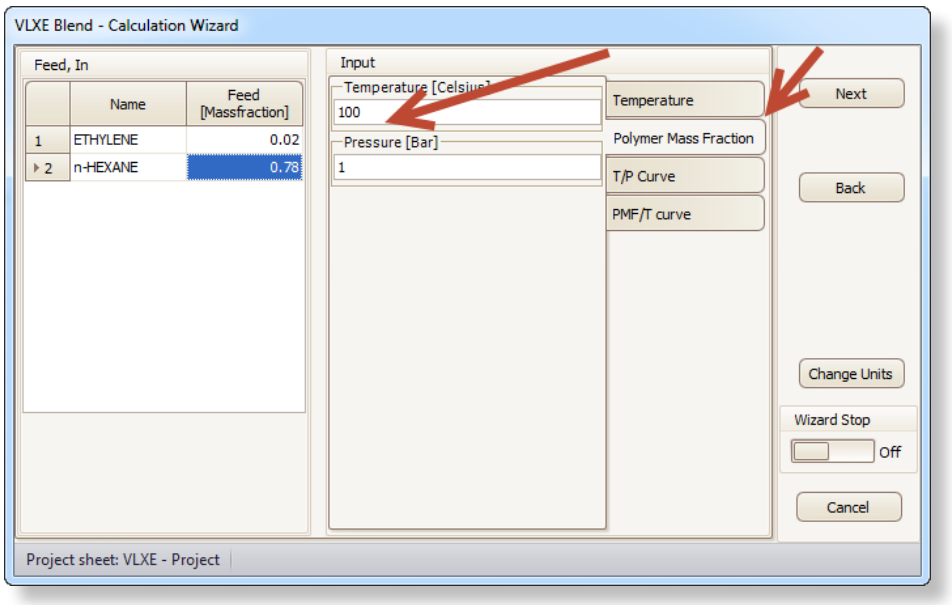
The result is shown below. Below the curve a solid phase forms, while above the curve it doesn´t. Note how little the curve changes with respect to changes in the polymer mass fraction in the mixture.



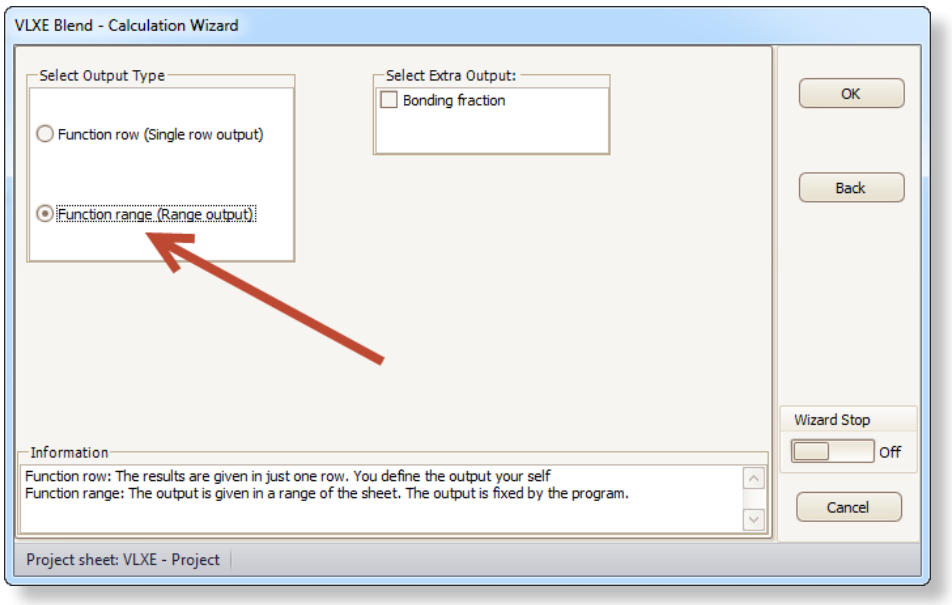
6.8.4 Polymer Mass Fraction

This will calculate the polymer mass fraction where a solid phase is formed at a fixed temperature and pressure. Once the temperature range from the PMF/T curve is known, the polymer mass fraction can be calculated. It is recommended to perform a PMF/T calculation before this calculation, doing so will provide an approximate temperature value. If the temperature is defined as being outside the maximum limit, then no solution will be found.

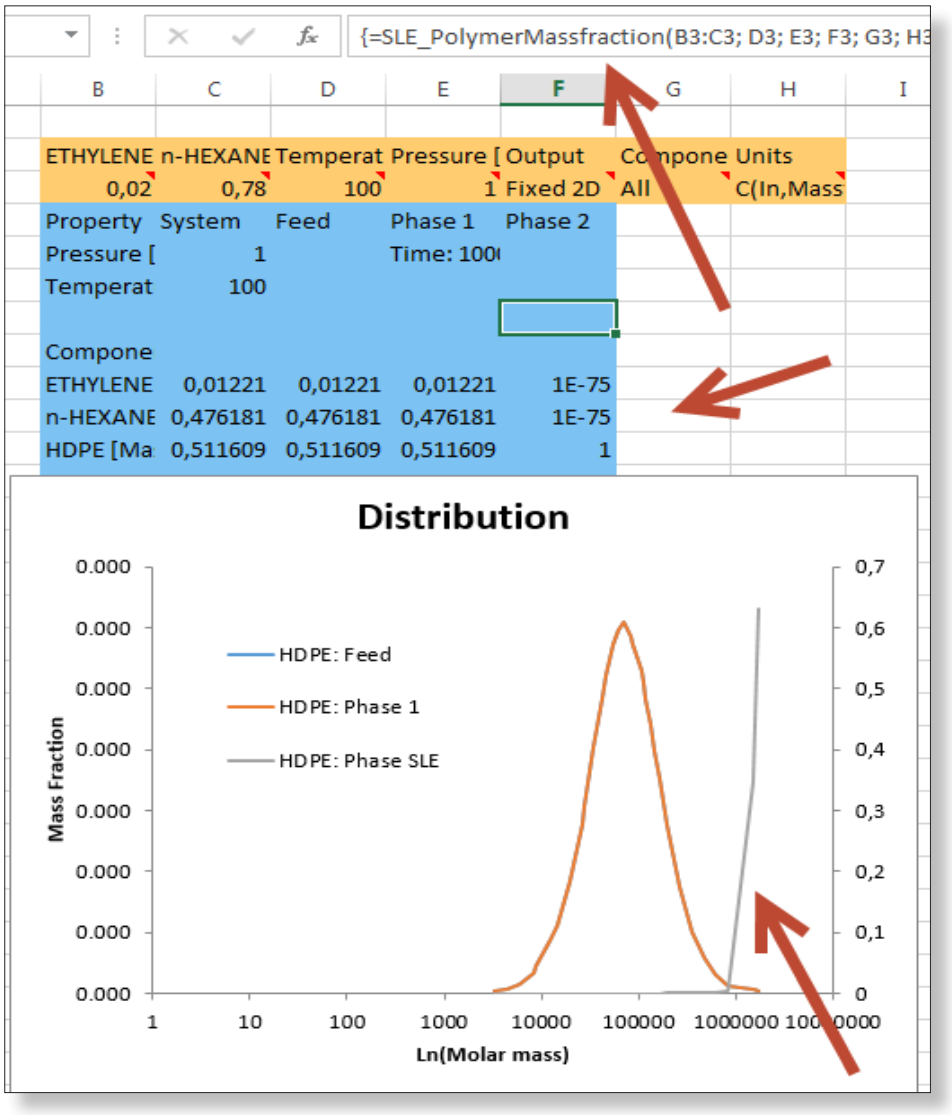
Create the calculation as before, using the input as shown below. However, make sure to select “Function Range” as output.



Select function range (range output) and click “OK”.



In the result below note how only polymer is in the heavy phase. Also note how VLXE Blend calculates the distribution and how only the heavy pseudo components are in the solid phase.

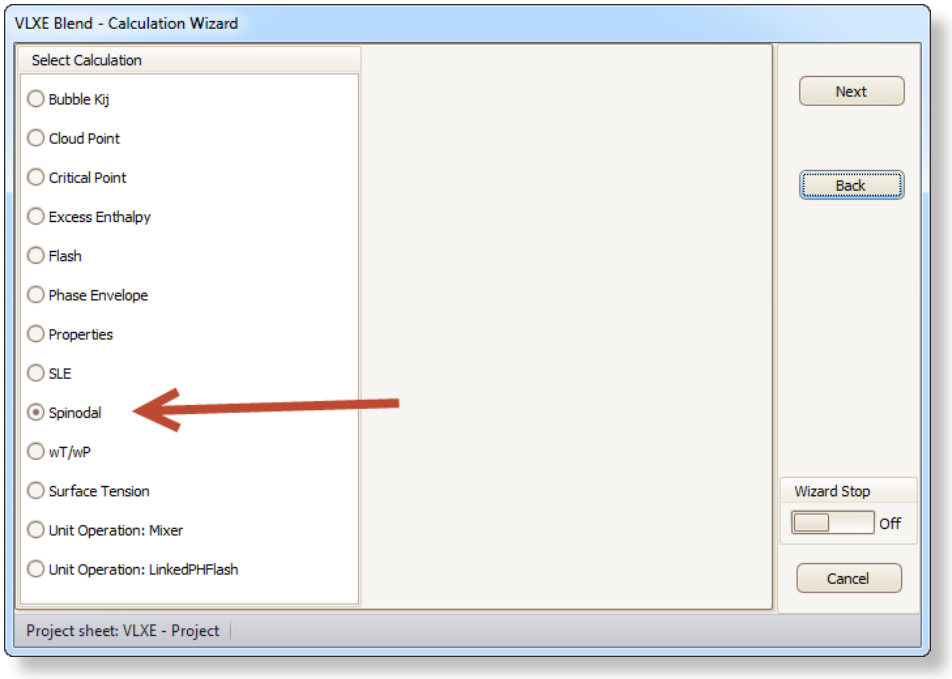


6.9 Spinodal

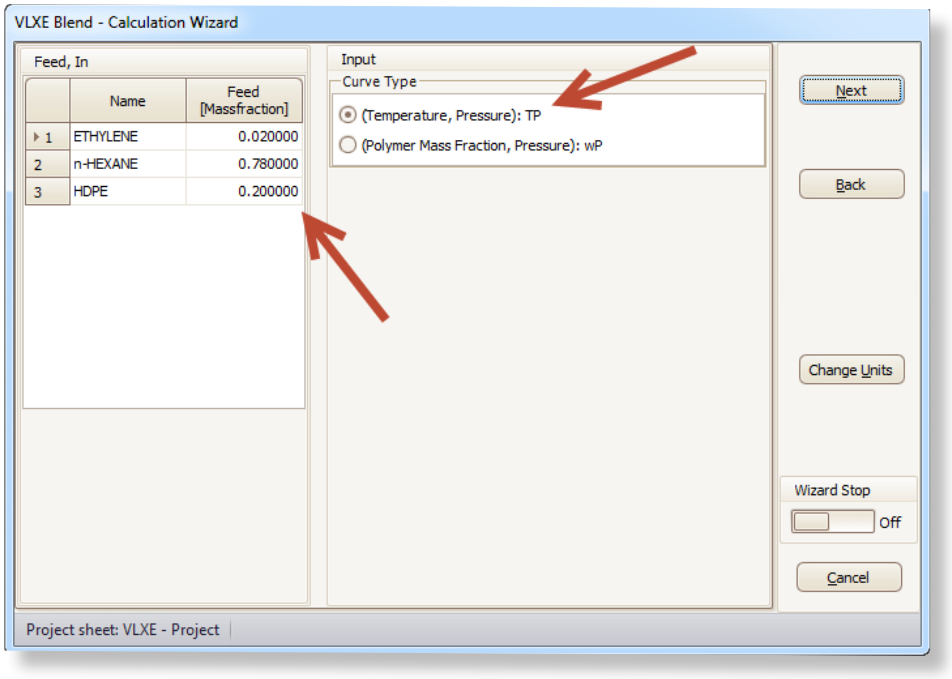
During the separation of components it is important to have an idea about the spinodal curve. VLXE Blend calculates the Spinodal for all supported systems. With the given thermodynamic model of system, one can calculate the set of compositions which form the boundary between the metastable and the truly unstable compositions. This set of compositions, which form a curve within the two phase area, is called the Spinodal curve.

The Spinodal is also handy if a new system is completly unknown; for polymer systems the Spinodal is often close to the phase boundary, so knowing the Spinodal gives a very good idea of the phase envelope.

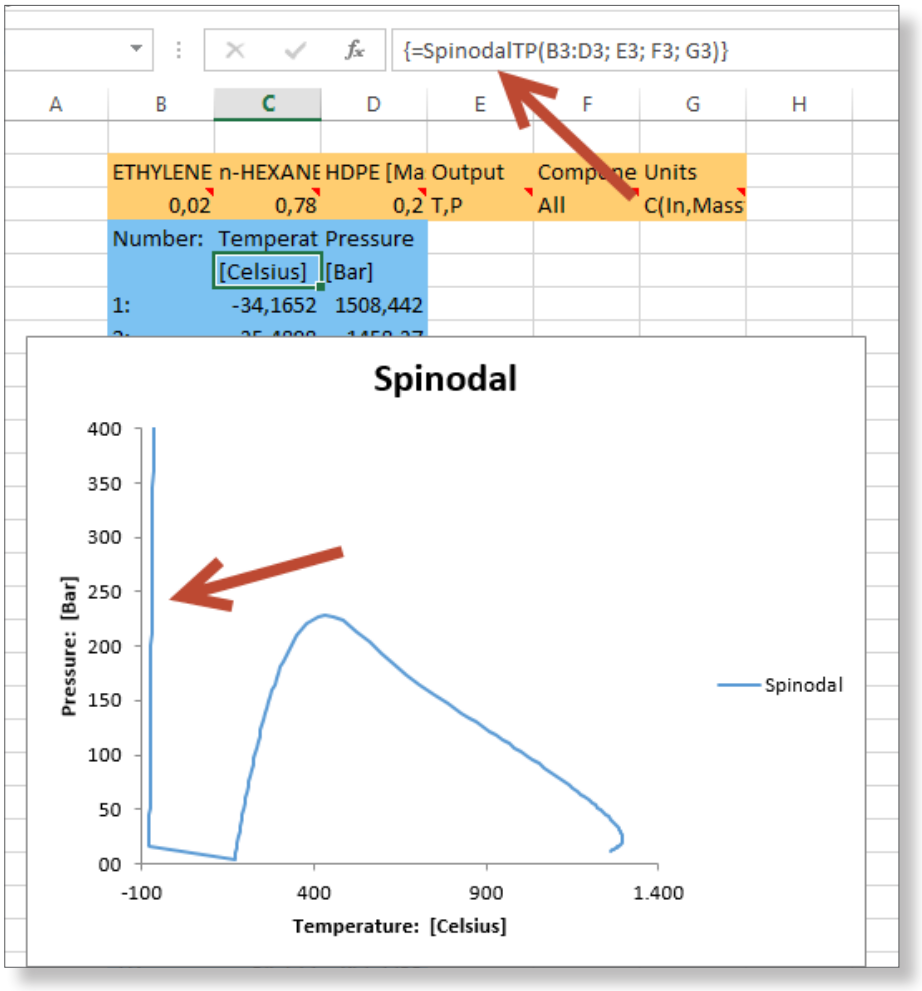
Select “Calculations” on the VLXE Blend ribbon. Select “Spinodal” as calculation and select “Next”.



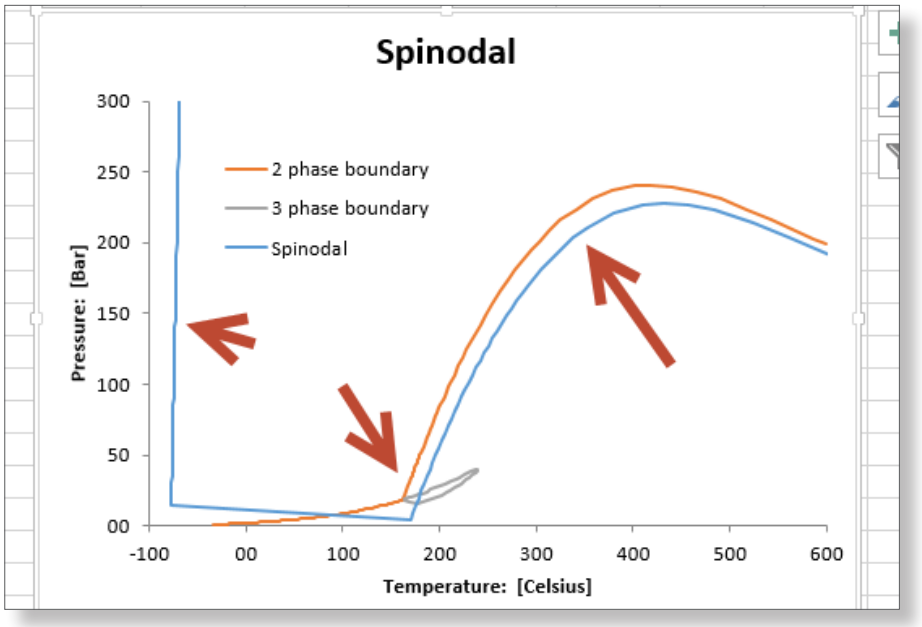
Enter Feed and select “Temperature, Pressure“ as the Spinodal type.
Select “Next” and then “OK” using the default output.



The Spinodal result is shown below. Note how it has an almost vertical line at lower pressures. The lower temperatue curve will continue to a very high pressure, as illustrated here.



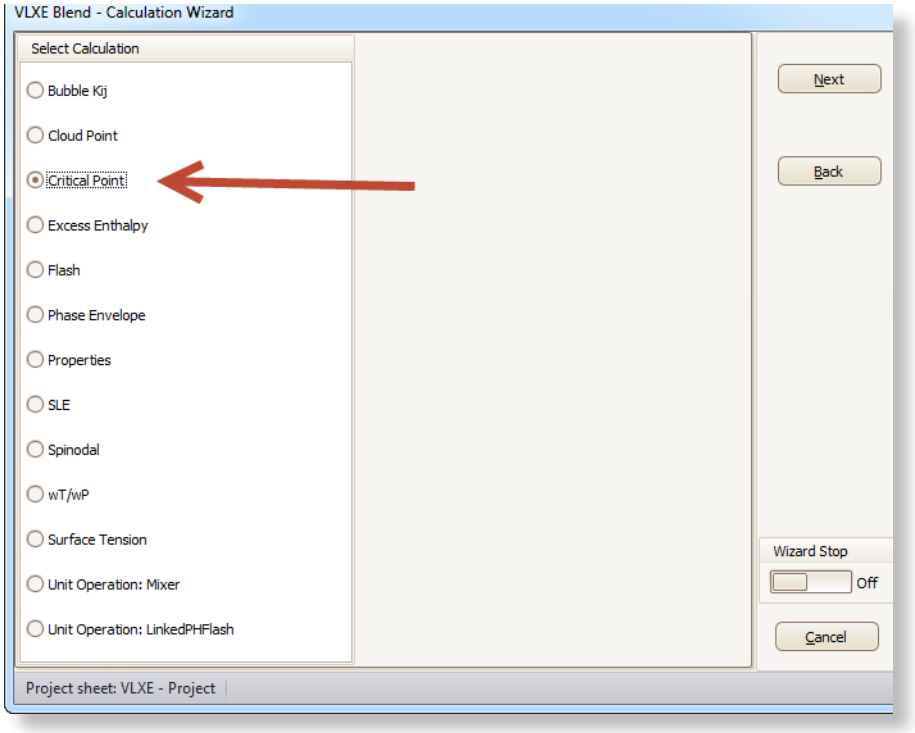
The best way to see the Spinodal is in combination with the phase envelope, as shown below. Note how close the Spinodal is to the phase boundary and how it does not detect the 3 phase area.



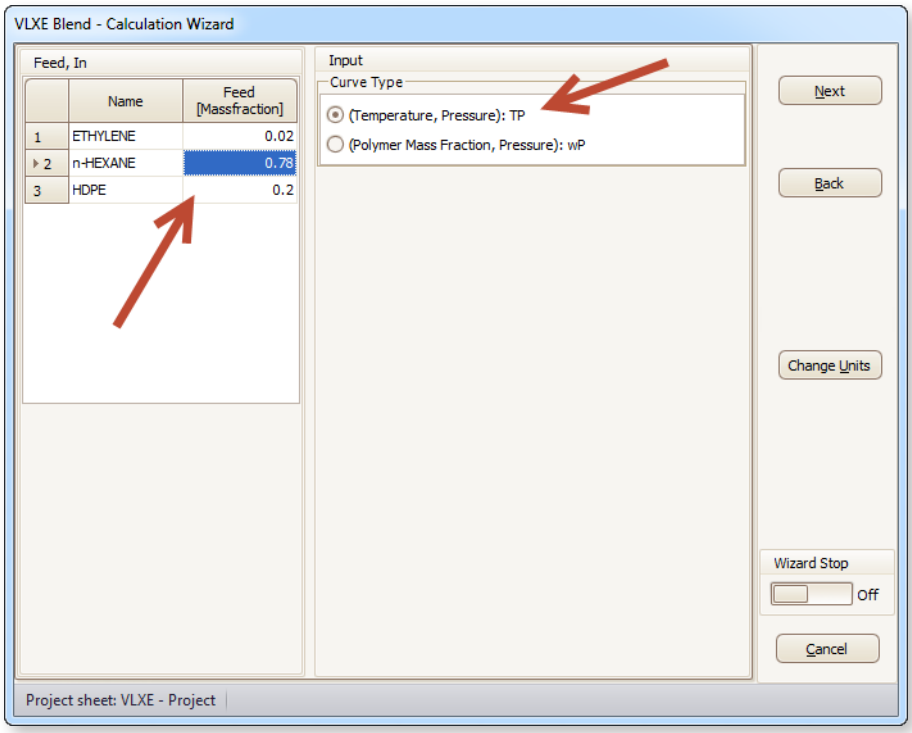
6.10 Critical Point

Critical point specifies the conditions (temperature, pressure) in which the liquid state of matter ceases to exist. It is also known as “Critical State”. VLXE Blend can calculate the critical point for all supported systems. Note that a system may not have a critical point, or that it may have multiple critical points.

Select “Calculation” on the VLXE Blend ribbon. Leave all components in and under calculations, select “Critical Point”.

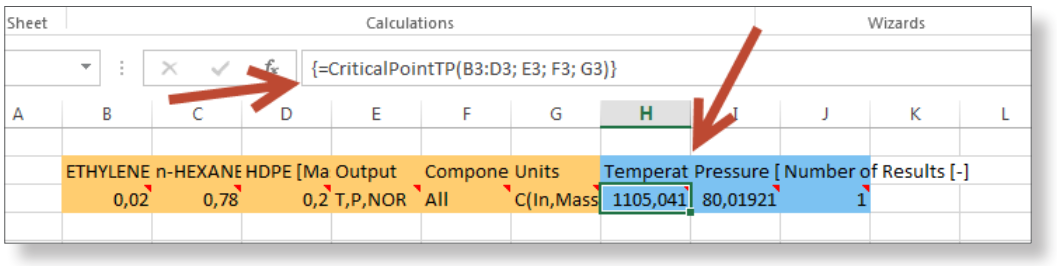


Select “Next” and now select “Temperature, Pressure” critical point.



Select function row (single row output) as an output. On the next page simply select “OK”, using the default output.

Critical temperature, pressure and number of critical points are calculated and are given below. For this solvent/polymer system with a given feed composition there is only one critical point. Note that the location of the single critical point is far outside the physical region.

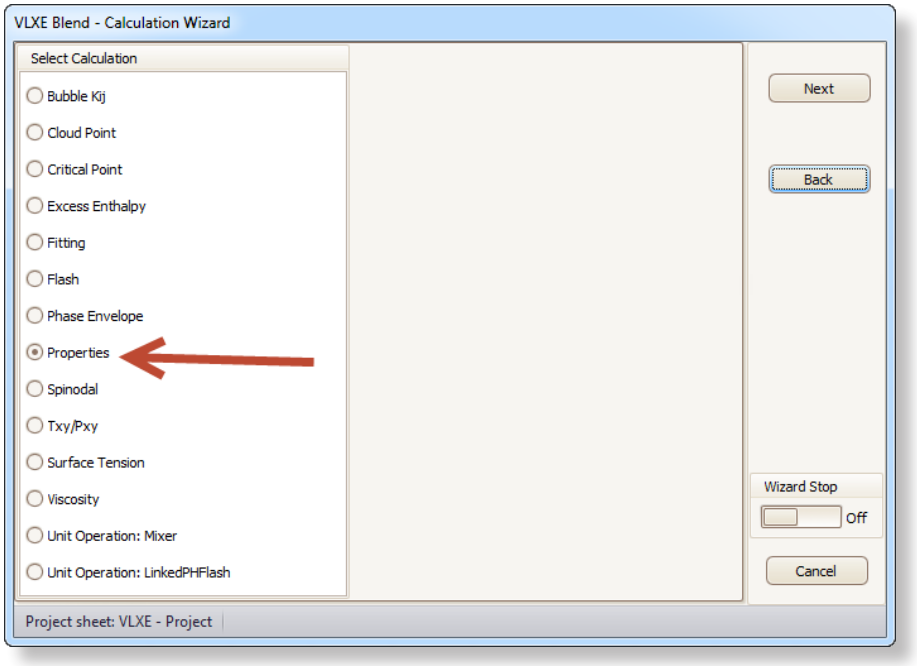


7) Properties

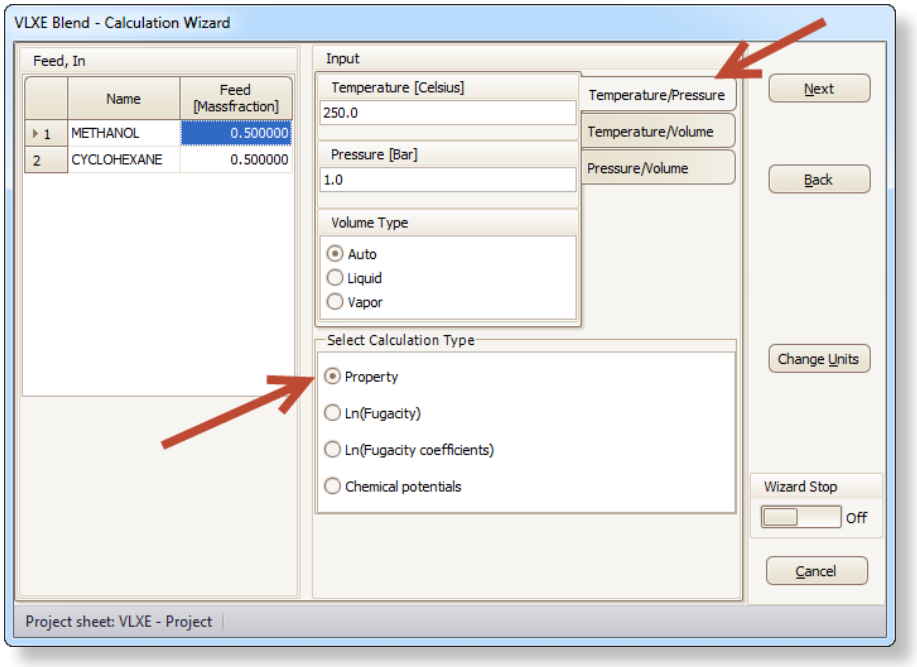
All the properties like: temperature, pressure, enthalpy entropy, heat capacity, compressibility factor, molecular weight etc. can be calculated with VLXE Blend. Both standard properties, like fugacy values including analytical derivatives for example, can be obtained. We will use the methanol/cyclohexane system from before as an example.

7.1 Standard Properties

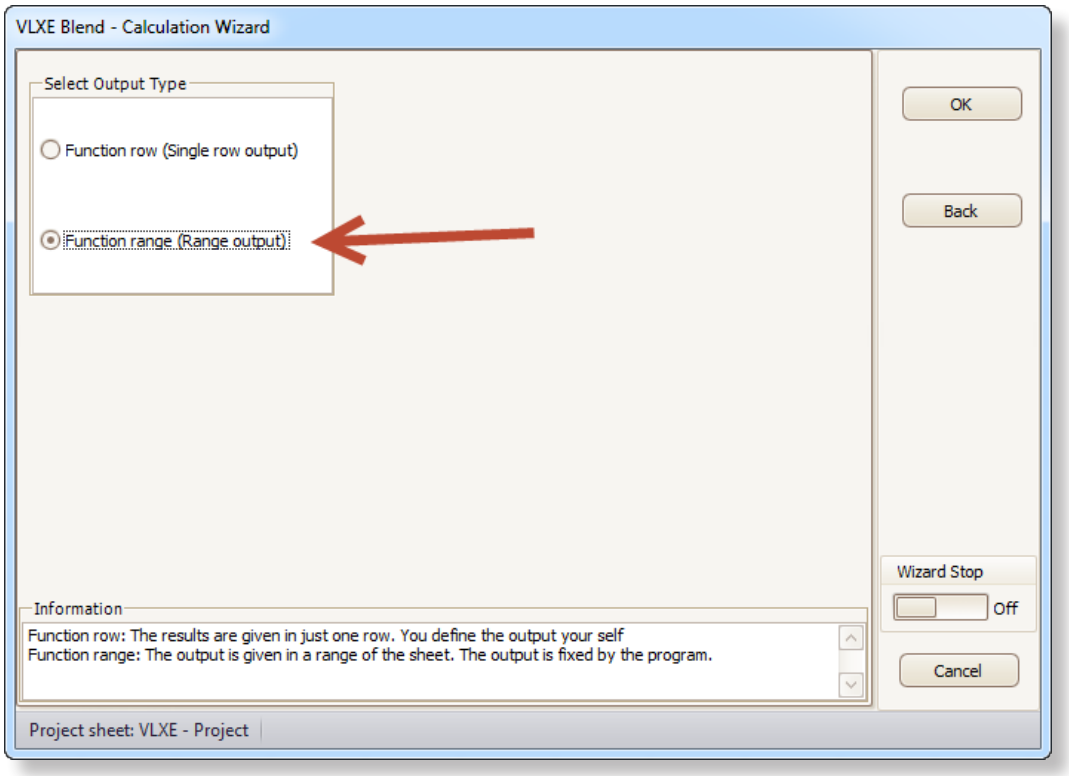
Select “Properties” in the calculation wizard.



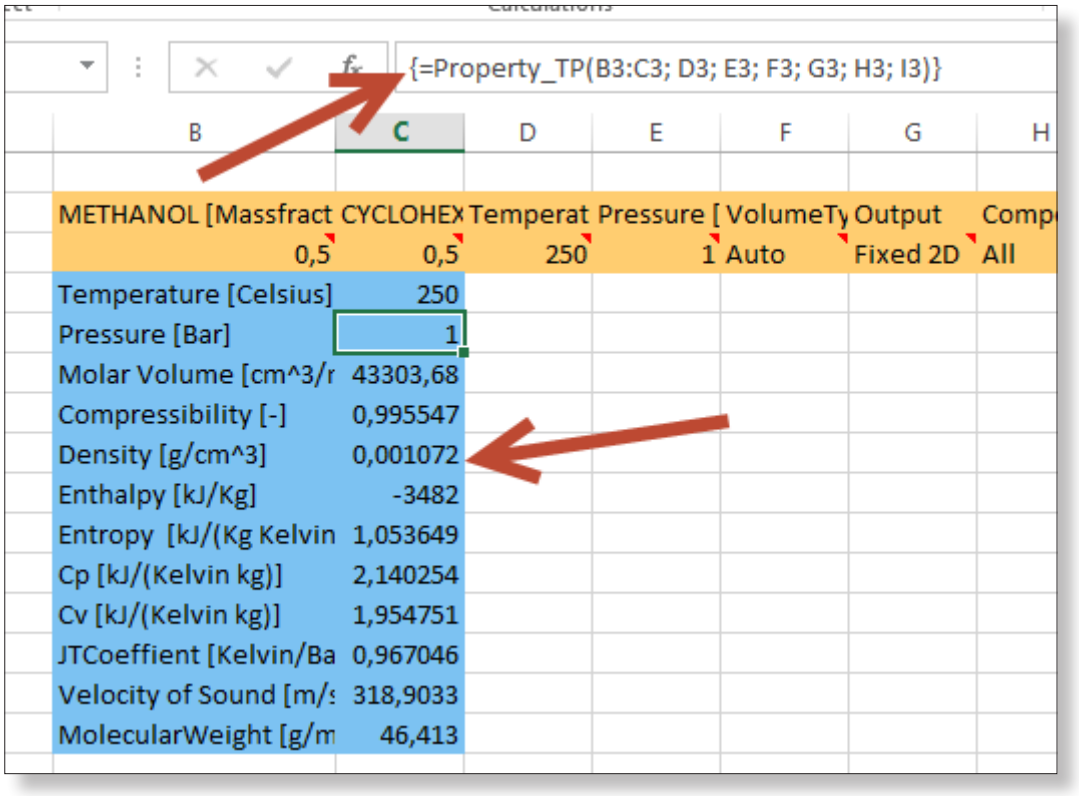
Select “Properties” as “Calculation type” and “Temperature/Pressure” as the variable. Note how VLXE Blend allows all 3 possible combinations of Temperature/Pressure/Volume.



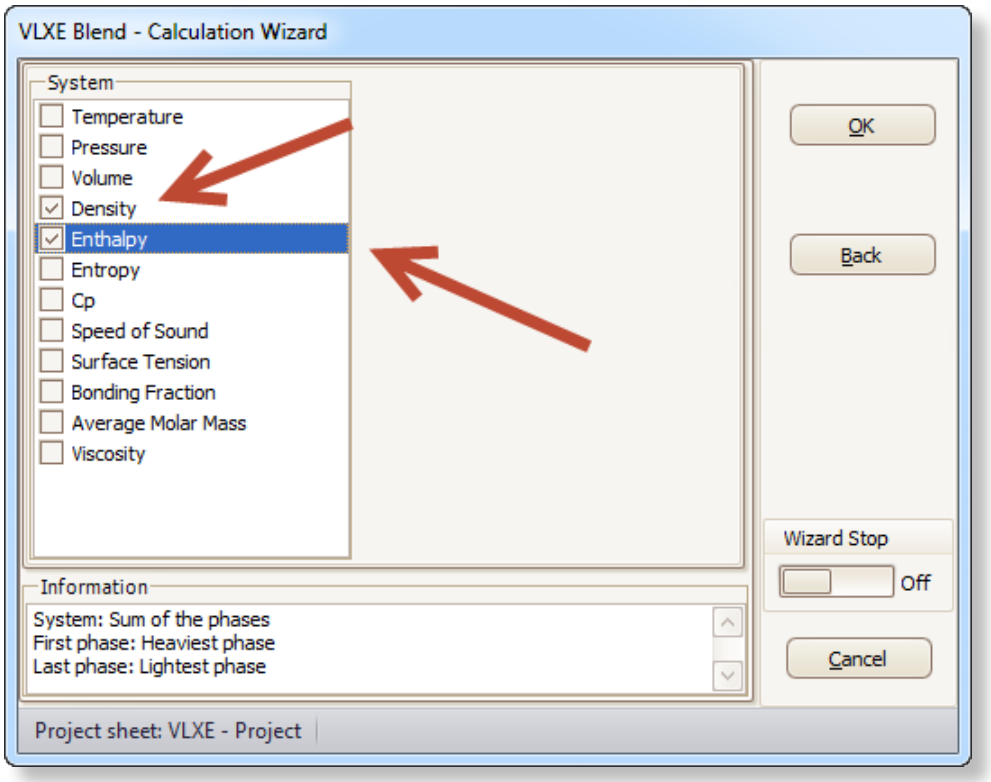
3. Click “Next” and there are two options to select output type. Here “Function range (Range output)” is selected and then click “OK”.



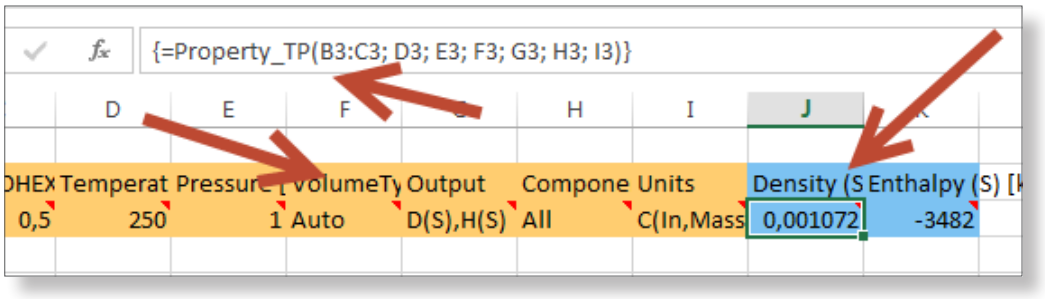
4. All the fixed temperature and pressure properties are calculated in an Excel spreadsheet.



5. In a similar way the result from function row requires an additional step. Select “Function row (single row output)” from step 3 above and click “Next”.

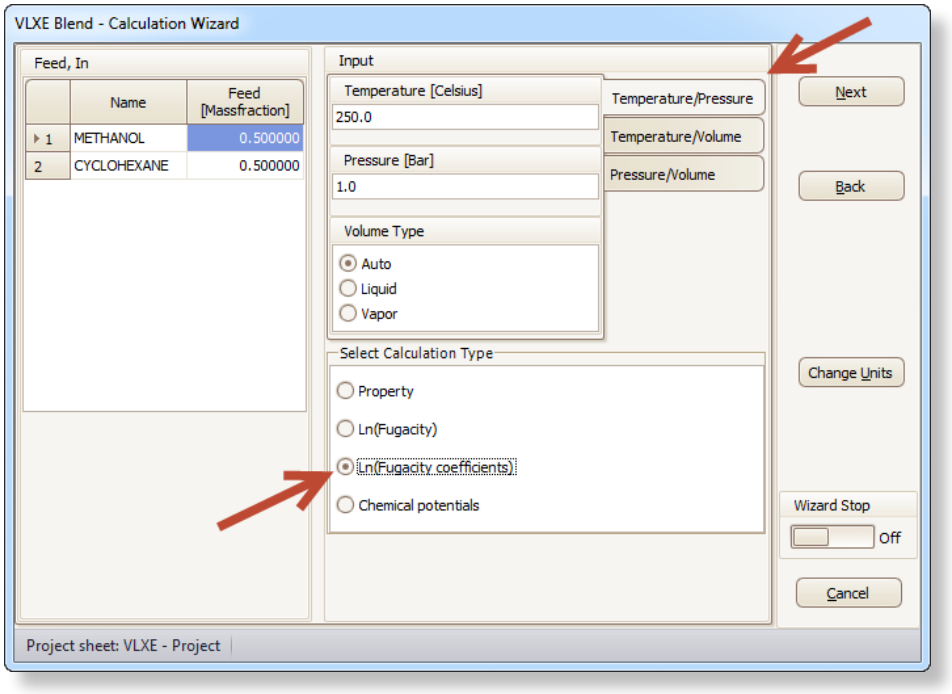


6. Click “OK” and the density at a fixed temperature and pressure is calculated and is shown in a blue cell, see below. Now by a simple Copy/Paste inside Excel this can be calculated over an entire temperature, pressure or/and composition range.

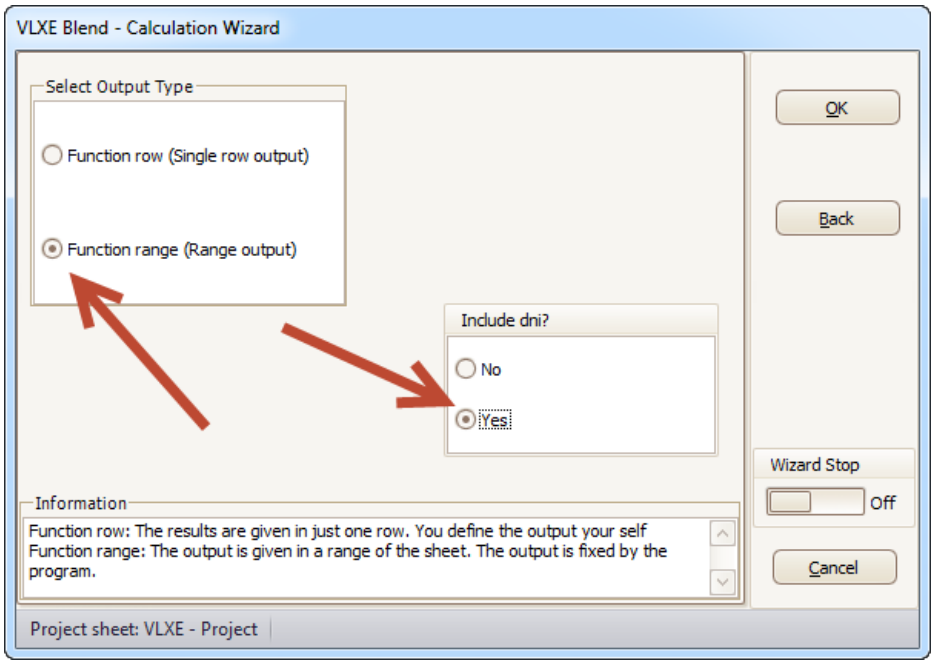


7.2 Lnfugacity Coefficients

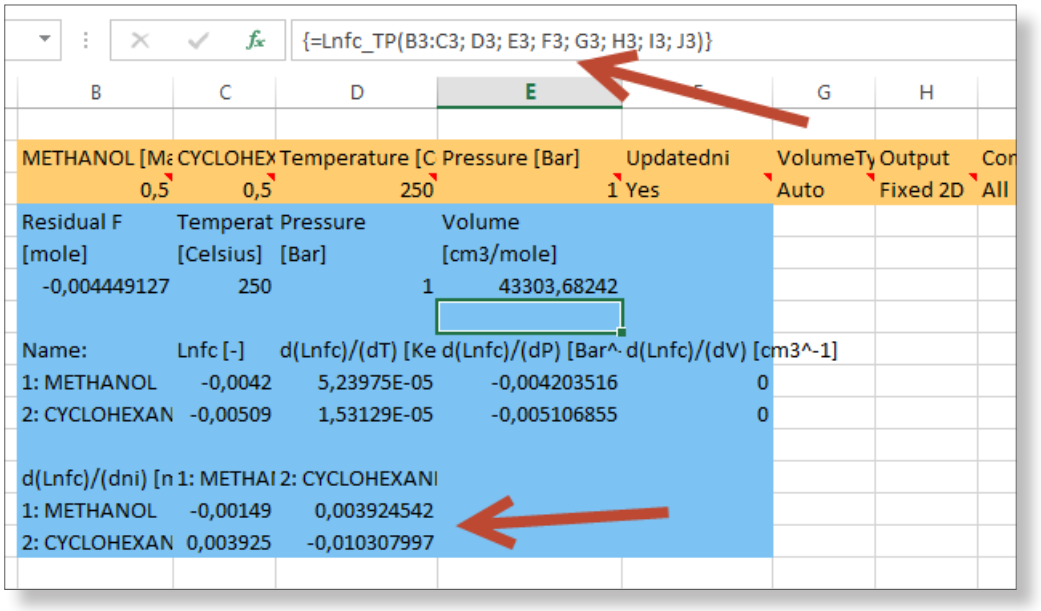
Internal properties like fugacity can also be calculated. Use the same steps as before, but now select ln (Fugacity coefficients) and then “Next”.



Select “Function range” as output plus “Include dni” which are the analytial derivatives of the LnFc with respect to mole numbers and click “OK”.



The result is shown below. Note how all relevant derivatives are included.
Please note that they are always given in internal units: Mole, bar, Kelvin and cm3.



Appendix A

How Goal Seek works:

With this function, you can find a desired value for a formula in one cell by calling a different cell that then affects the first cell.

Define and solve a problem by using Goal Seek

1. On the Data ribbon, select “What-If Analysis”, in the dropdown select “Goal Seek”.

2. In the “Set Cell” box, enter a cell reference or name for the Set Cell. The Set Cell must contain a formula.

3. To have the Set Cell be a certain value, click “To Value”, and then type the value in the box.

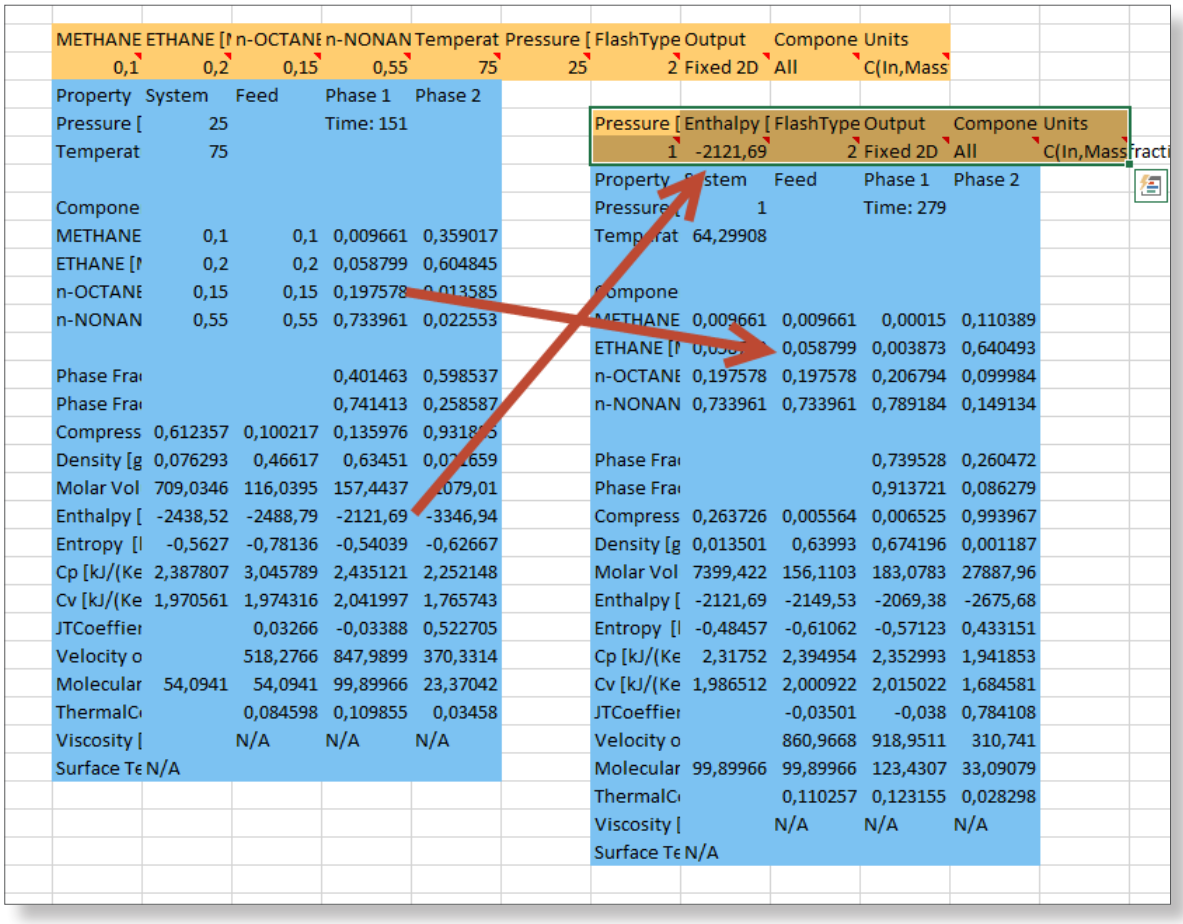
4. In the “By Changing Cell” box, enter a name or reference for the adjustable cell, the adjustable cell must be related directly or indirectly to the Set Cell.

5. Click “OK” to get the desired results.

Example

To understand this in a better way lets take a simple example.

1. We have an isenthalpic system, where we link 2 PH flash calculations. The feed and enthalpy are taken from the heavy phase from the first flash, see below. Note how the composition and enthalpy for the second flash is taken from the first flash calculation.



METHANE	ETHANE [I	n-OCTANE	n-NONAN	Temperat	Pressure [	FlashType	Output	Compone	Units
0,1	0,2	0,15	0,55	75	25	2	Fixed 2D	All	C(In,Mass

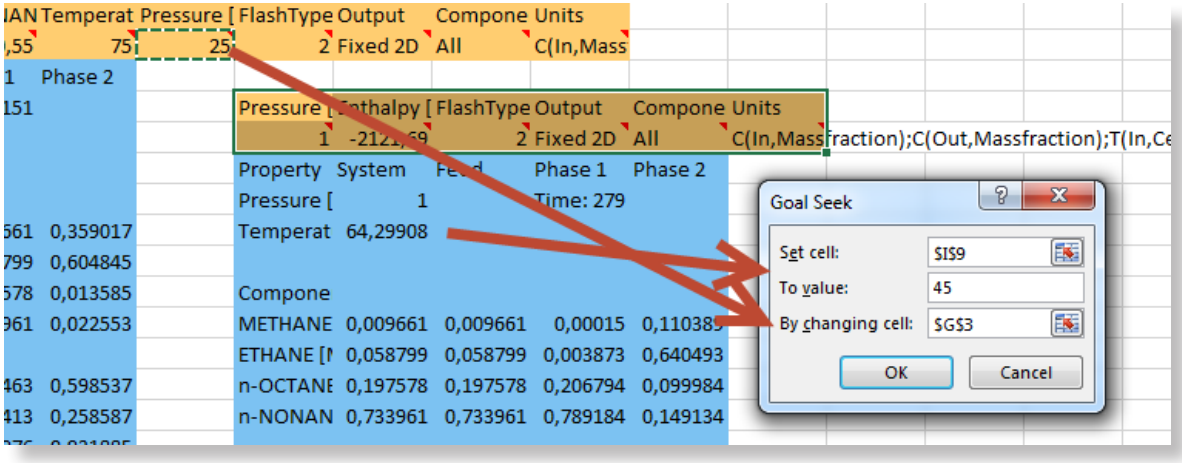
Property	System	Feed	Phase 1	Phase 2
Pressure [	25		Time: 151	
Temperat	75			
Compone				
METHANE	0,1	0,1	0,009661	0,359017
ETHANE [I	0,2	0,2	0,058799	0,604845
n-OCTANE	0,15	0,15	0,197578	0,013585
n-NONAN	0,55	0,55	0,733961	0,022553
Phase Frac			0,401463	0,598537
Phase Frac			0,741413	0,258587
Compress	0,612357	0,100217	0,135976	0,931835
Density [g	0,076293	0,46617	0,63451	0,021659
Molar Vol	709,0346	116,0395	157,4437	1079,01
Enthalpy [	-2438,52	-2488,79	-2121,69	-3346,94
Entropy [I	-0,5627	-0,78136	-0,54039	-0,62667
Cp [kJ/(Ke	2,387807	3,045789	2,435121	2,252148
Cv [kJ/(Ke	1,970561	1,974316	2,041997	1,765743
JTCoeffier		0,03266	-0,03388	0,522705
Velocity o		518,2766	847,9899	370,3314
Molecular	54,0941	54,0941	99,89966	23,37042
ThermalC		0,084598	0,109855	0,03458
Viscosity [		N/A	N/A	N/A
Surface Te	N/A			

Pressure [	Enthalpy [	FlashType	Output	Compone	Units
1	-2121,69	2	Fixed 2D	All	C(In,Mass fracti

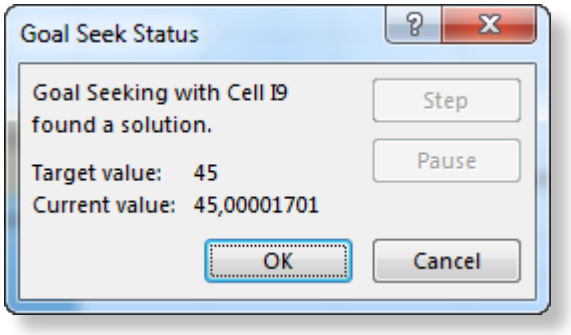
Property	System	Feed	Phase 1	Phase 2
Pressure [	1		Time: 279	
Temperat	64,29908			
Compone				
METHANE	0,009661	0,009661	0,00015	0,110389
ETHANE [I	0,058799	0,058799	0,003873	0,640493
n-OCTANE	0,197578	0,197578	0,206794	0,099984
n-NONAN	0,733961	0,733961	0,789184	0,149134
Phase Frac			0,739528	0,260472
Phase Frac			0,913721	0,086279
Compress	0,263726	0,005564	0,006525	0,993967
Density [g	0,013501	0,63993	0,674196	0,001187
Molar Vol	7399,422	156,1103	183,0783	27887,96
Enthalpy [	-2121,69	-2149,53	-2069,38	-2675,68
Entropy [I	-0,48457	-0,61062	-0,57123	0,433151
Cp [kJ/(Ke	2,31752	2,394954	2,352993	1,941853
Cv [kJ/(Ke	1,986512	2,000922	2,015022	1,684581
JTCoeffier		-0,03501	-0,038	0,784108
Velocity o		860,9668	918,9511	310,741
Molecular	99,89966	99,89966	123,4307	33,09079
ThermalC		0,110257	0,123155	0,028298
Viscosity [		N/A	N/A	N/A
Surface Te	N/A			

2. The goal is to adjust the pressure of the first flash in order to obtain a temperature of 45°C in the second flash.

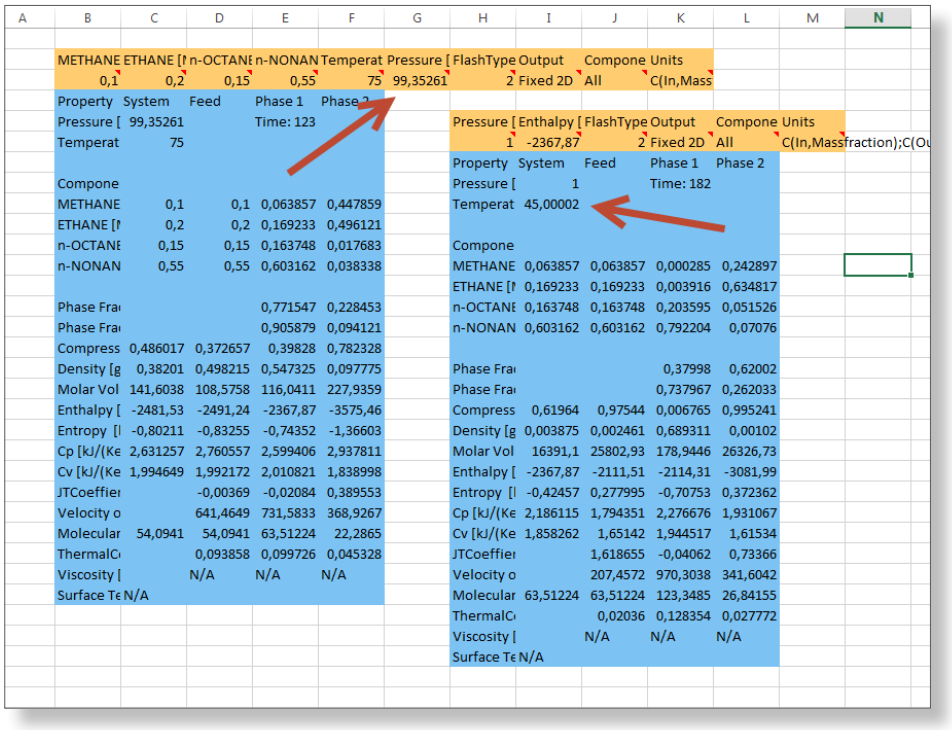
3. Open "Goal Seek" and link the cells as shown below. Then click "OK".



Goal seek will then run for a few seconds before it finds a solution. See below



4. The desired results are obtained and are shown below.



METHANE	ETHANE [I	n-OCTANE	n-NONAN	Temperat	Pressure [	FlashType	Output	Compone	Units
0,1	0,2	0,15	0,55	75	99,35261	2	Fixed 2D	All	C(In,Mass

Property	System	Feed	Phase 1	Phase 2
Pressure [	99,35261		Time: 123	
Temperat	75			
Compone				
METHANE	0,1	0,1	0,063857	0,447859
ETHANE [I	0,2	0,2	0,169233	0,496121
n-OCTANE	0,15	0,15	0,163748	0,017683
n-NONAN	0,55	0,55	0,603162	0,038338
Phase Frai			0,771547	0,228453
Phase Frai			0,905879	0,094121
Compress	0,486017	0,372657	0,39828	0,782328
Density [g	0,38201	0,498215	0,547325	0,097775
Molar Vol	141,6038	108,5758	116,0411	227,9359
Enthalpy [	-2481,53	-2491,24	-2367,87	-3575,46
Entropy [I	-0,80211	-0,83255	-0,74352	-1,36603
Cp [kJ/(Ke	2,631257	2,760557	2,599406	2,937811
Cv [kJ/(Ke	1,994649	1,992172	2,010821	1,838998
JTCoeffier		-0,00369	-0,02084	0,389553
Velocity o		641,4649	731,5833	368,9267
Molecular	54,0941	54,0941	63,51224	22,2865
ThermalC		0,093858	0,099726	0,045328
Viscosity [		N/A	N/A	N/A
Surface Te	N/A			

Pressure [	Enthalpy [	FlashType	Output	Compone	Units
1	-2367,87	2	Fixed 2D	All	C(In,Massfraction);C(Ou

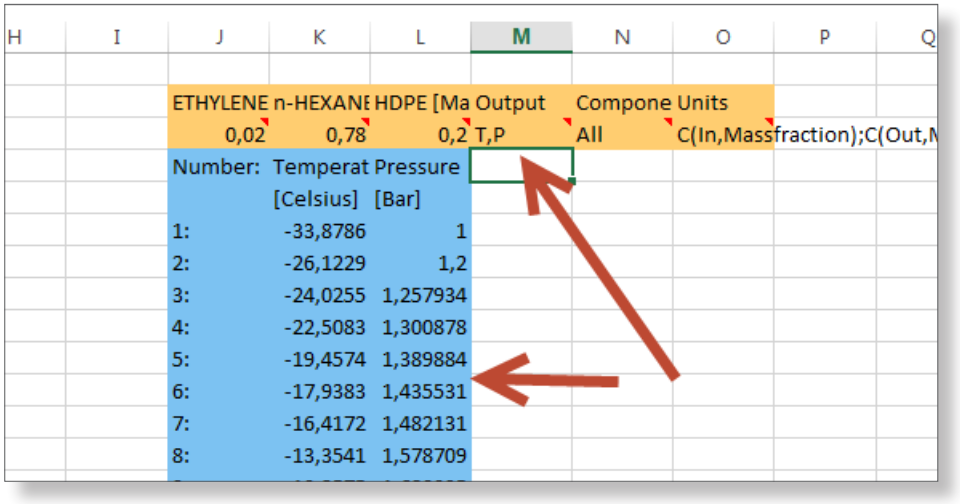
Property	System	Feed	Phase 1	Phase 2
Pressure [	1		Time: 182	
Temperat	45,00002			
Compone				
METHANE	0,063857	0,063857	0,000285	0,242897
ETHANE [I	0,169233	0,169233	0,003916	0,634817
n-OCTANE	0,163748	0,163748	0,203595	0,051526
n-NONAN	0,603162	0,603162	0,792204	0,07076
Phase Frai			0,37998	0,62002
Phase Frai			0,737967	0,262033
Compress	0,61964	0,97544	0,006765	0,995241
Density [g	0,003875	0,002461	0,689311	0,00102
Molar Vol	16391,1	25802,93	178,9446	26326,73
Enthalpy [	-2367,87	-2111,51	-2114,31	-3081,99
Entropy [I	-0,42457	0,277995	-0,70753	0,372362
Cp [kJ/(Ke	2,186115	1,794351	2,276676	1,931067
Cv [kJ/(Ke	1,858262	1,65142	1,944517	1,61534
JTCoeffier		1,618655	-0,04062	0,73366
Velocity o		207,4572	970,3038	341,6042
Molecular	63,51224	63,51224	123,3485	26,84155
ThermalC		0,02036	0,128354	0,027772
Viscosity [		N/A	N/A	N/A
Surface Te	N/A			

Appendix B

How to Work with Array formulas

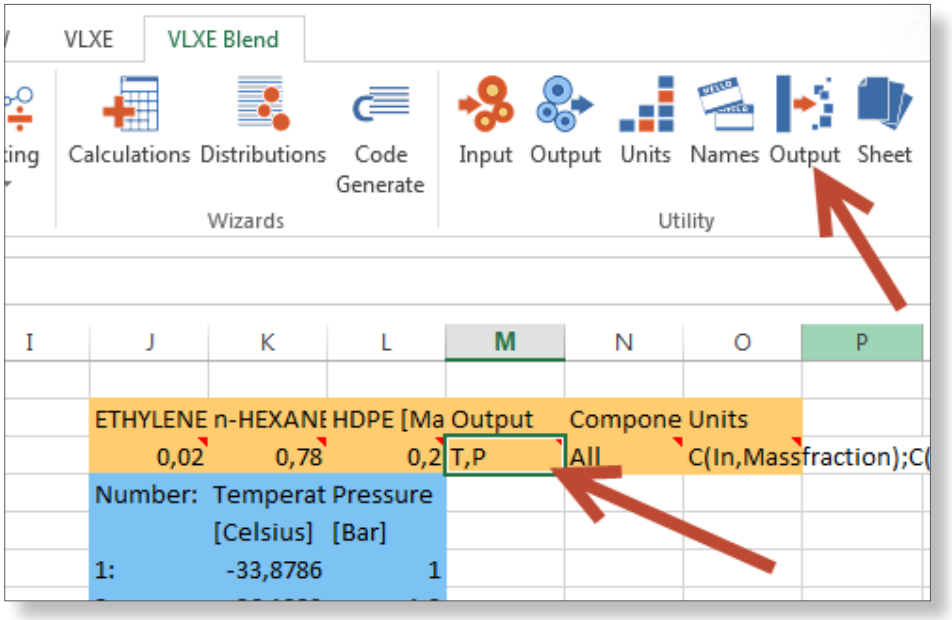
What are array formulas?
This is a Excel feature and is used extensively by VLXE Blend. It is simply a function call that gives output in more than one cell.

The use of an array function is explained with a phase envelope calculation. The method used will apply to any array function in Excel.
The figure below shows output in terms of temperature and pressure.

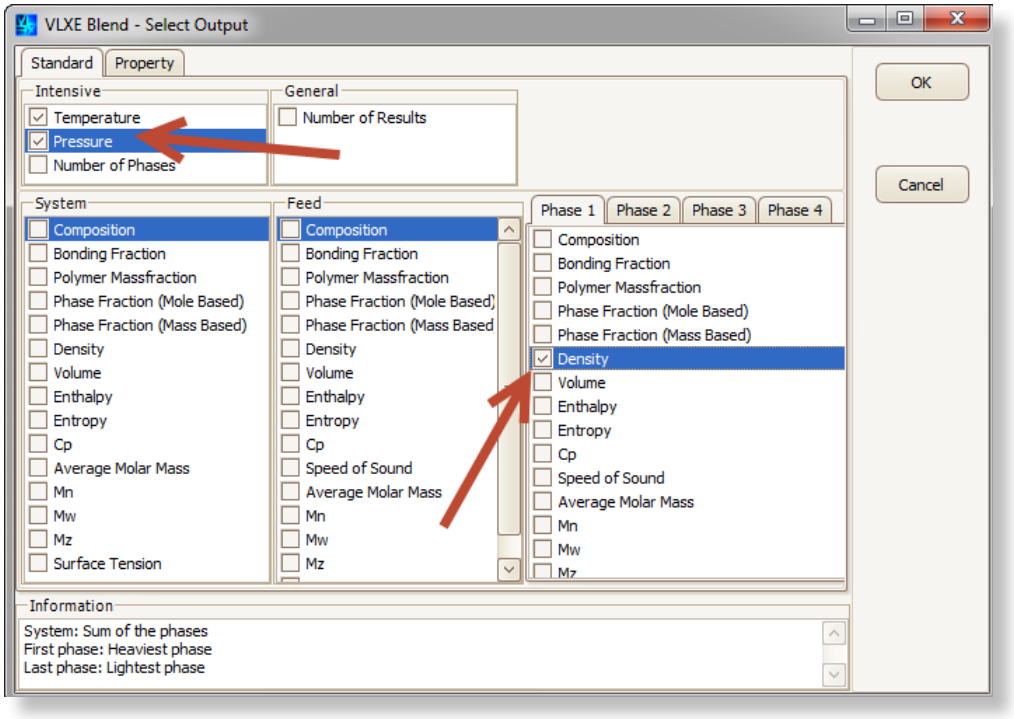


Now we want to change the calculation so that density for the heavy phase becomes part of the output. In order to do this we have to expand the output area by one column more and additionally change the output argument of the function. Plus we have to change the output argument so this density is part of the result.

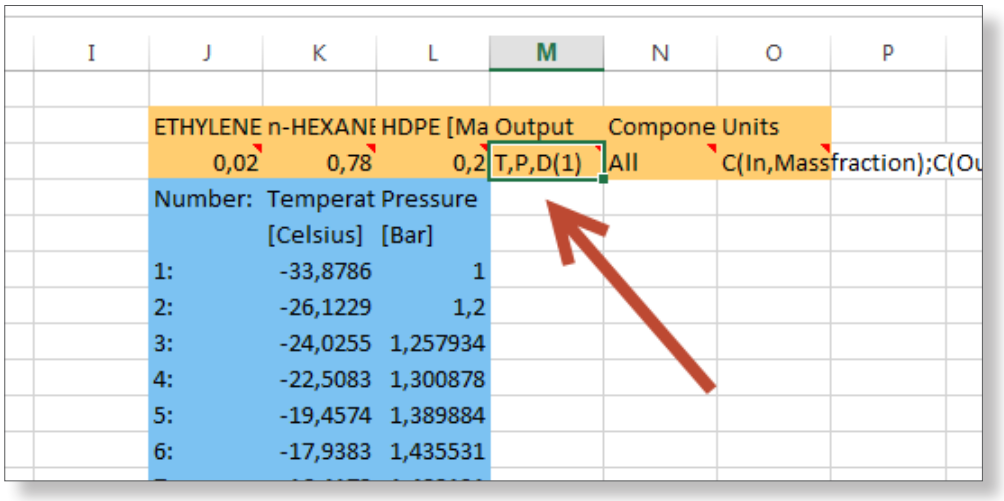
First we change the output. Select the cell that contains the output argument and select “Output” on the VLXE Blend ribbon.



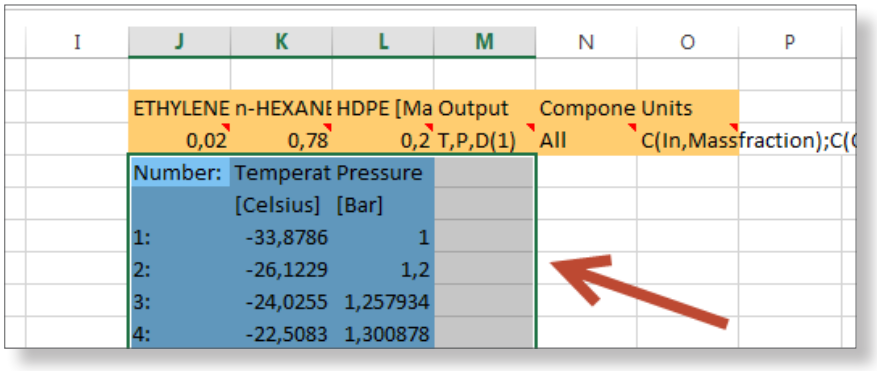
Change the output by selecting the density for phase 1.



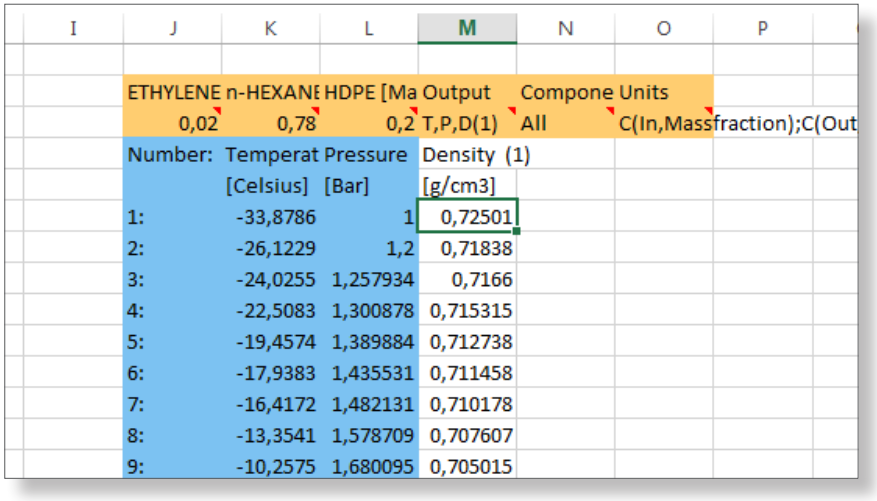
The selected density is now part of the Output. Note how the output area is too small to show the new values.



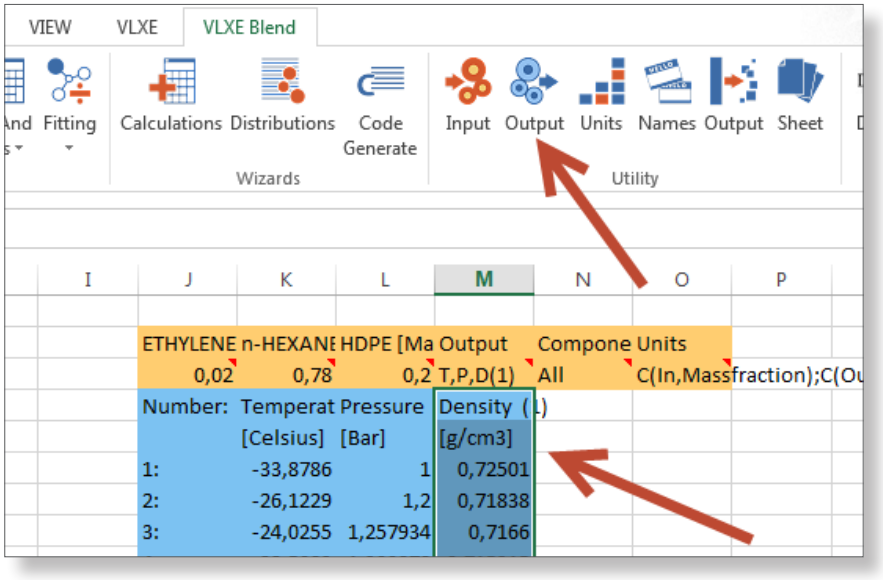
To expand the output area, select all the current output cell plus the next column (the blue area plus the column to the right).



Click in the formula bar and press Ctrl+Shift+Enter. The function is then recalculated and the output range extended over the entire selected range in the sheet. Density is now included in the output.



The new output cell does not have the correct color. So to make things look consistent, select it and then click on “Output” in the VLXE Blend Ribbon.



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